CALCULATION OF ELECTRON SCATTERING CROSS SECTIONS FOR CARBON-TWELVE AND LITHIUM-SIX USING PHASE SHIFT ANALYSIS

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THESIS

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ABSTRACT

A phase shift analysis is used to obtain scattering cross sections for incident electrons on Carbon-12 and Lithium-6. Results are given for incident electron energies of 10-100 Mev and for scattering angles of 45, 90 and 135 degrees A gaussian p-shell charge distribution is used for Carbon-12, and an empirical charge distribution developed by L R. Suelzle is used for Lithium-6. A comparison is also made between the phase-shift results and results obtained using the Born approximation.

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I. INTRODUCTION

Many experiments on the elastic scattering of high energy electrons from nuclei have been conducted in an effort to understand the structure of the nuclei. That the nuclear charge distribution has finite extension has been clearly exhibited [1, 2]. The exact form of this charge distribution is not known, although many theoretical and empirical models have been proposed. From experiments, it has been tentatively concluded that this charge distribution peaks at the center of the nucleus, and tapers off at the edge. This conclusion is reached using the Born approximation, which is most accurate for light nuclei.

The fact that the Born approximation is not accurate for heavy elements led Yennie, Ravenhall and Wilson [3] to carry out a phase shift analysis of the scattering process. This analysis neglected the mass of the electron, which is a good approximation for very high energy electrons. Another phase shift analysis by Rawitscher [4] did not make this approximation and is therefore apparently a more accurate calculation. It is the phase shift analysis by Rawitscher which forms the basis for this work.

The model used for this "exact" phast shift analysis is the Dirac equation for an electron in the electrostatic potential of a static, spherically symmetric charge distribution. The interaction of the electron with nuclear magnetic or electric quadrupole moments, and possible nuclear excitation is neglected in this analysis. Calculations done by Schiff [6] using the first Born approximation suggest that the magnetic quadrupole moment interaction is negligible at high energies, and reference [3] suggests that the electric quadrupole moment and nuclear excitation interactions are negligible except for a few particular elements at large angles.

The electron scattering experiments conducted at this facility are of relatively low energy, 20 - 100 Mev, when compared to energies available at other linear accelerators. For this given range of energy, and for light nuclei, the Born approximation should provide a good method for calculation of scattering cross sections. A comparison of results, using the Born approximation and phase shift analysis, for light nuclei is given in Section III. The computer program which accomplishes the desired calculations is contained herein following Appendix A. All calculations were done on the IBM 360 computer available at this facility. The program is written in FORTRAN and comments are located in various sections to aid in understanding.

II. METHOD OF CALCULATION

The well-known Dirac equation forms the basis of the calculations, and it is from it that the scattered wave function is obtained by the method of partial wave expansion [5]. As was stated earlier, the potential acting on the electron is assumed to be entirely the result of a static Coulomb interaction arising from a charge distribution $\rho(r)$.

The program has built into it many different forms for $\rho(r)$. Those used for calculation of results in Section III are shown below:

(1) gaussian p-shell:

$$\rho(r) = \rho_0 \left[1 + \alpha\left(\frac{r}{a}\right)^2\right] \exp\left[-\left(\frac{r}{a}\right)^2\right]$$

(2) Li^6:

$$\rho(r) = \frac{1}{8\pi^{3/2}}\left[\frac{1}{a^3}\exp\left(-\frac{r^2}{4a^2}\right) - \frac{c^2(6b^2 - r^2)}{4b^7}\exp\left(-\frac{r^2}{4b^2}\right)\right]$$

The second one above, (2), is an empirical form obtained from the work of Suelzle, Yearian, and Crannell [7]. In the above forms, r is the radial distance from the center of the nucleus. The potential inside the charge distribution may be calculated using the expression:

$$-V(r) = \frac{4\pi\left(\frac{Ze^2}{\hbar c}\right)}{r}\int_0^r e(r')r'^2\,dr' + 4\pi\left(\frac{Ze^2}{\hbar c}\right)\int_r^\infty e(r')r'\,dr'$$

while the potential outside the nucleus is of the form

$$V(r) = -\frac{Ze^2}{\hbar c r}$$

The scattering wave function, in the partial wave analysis, is regarded as a series of eigenfunctions of the operator k, which is related to the angular mimentum for Dirac Particles. (8). The radial wave functions $F_k(x)$ and $G_k(x)$ obey the radial equations:

$$\left(\frac{d}{dx} - \frac{k}{x}\right) g_k + (1 - v_1)\, f_k = 0$$

$$\left(\frac{d}{dx} + \frac{k}{x}\right) f_k - (1 - V_2)\, g_k = 0$$

where

$$G_k = r^{-1}(E + 1)^{\frac{1}{2}} g_k, \quad F_k = r^{-1}(E - 1)^{\frac{1}{2}} f_k$$

See Appendix A for explanation of symbols and further details. The asymptotic behavior of the F's and G's determines the phase shifts η_k from which $f(\theta)$ and $g(\theta)$ and finally the cross section is calculated

The integration of the above radial equations must be done numerically The method used is outlined in reference [3] It is essentially a step-by-step procedure based on derivatives rather than on differences, following formulas given in reference [9].

Starting with a regular solution obtained by a power series expansion about the origin [10], the radial equations are integrated from x = 1/1024 to a fitting radius x_o. From the Appendix, $x = r_o K$, where $K = mcp/\hbar$ and p = momentum/mc. At x_o, the $f_k(x_o)$ and $g_k(x_o)$ are fitted to two pairs of linearly independent Coulomb functions:

$$g_k(x_o) = C_k g_k^R(x_o) + D_k g_k^I(x_o)$$

$$f_k(x_o) = C_k f_k^R(x_o) + D_k f_k^I(x_o)$$

I, R refer to Coulomb functions which are regular (R) or irregular (I), at the origin

The major difference in the phase-shift analysis used here and the one developed by Yennie et al, shows up in the calculation of the phase shift η_k. Due to the inclusion of the rest mass of the electron in the total energy, the value of the phase shift for +k values is not equal to the phase shift of -k, and must be calculated separately.

The scattering amplitudes $f(\theta)$ and $g(\theta)$ are obtained from the phase shifts and Legendre polynomials by a summation procedure found satisfactory

in reference [3]. A change in the normal summation procedure was made to improve the convergence of the Coulomb scattering amplitude series.

The new summation procedure, that of reference [3], is designed to transform $f(\theta)$ to make it less singular at small values of θ. This is accomplished by multiplying $f(\theta)$ by a function which vanishes at $\theta = 0$ and then expanding the new function in a series of Legendre polynomials. First, $f(\theta)$ is represented by

$$2ikf = \sum c_k P_k(\cos \theta)$$

The mth reduced series is defined by:

$$(1 - \cos \theta)^m \, 2ikf = \sum c_k^{(m)} P_k(\cos \theta)$$

A similar set of expressions exists for $g(\theta)$ and can be found in Appendix A.

A value of $m = 3$ was used in reference [3] and reference [4]. In this work, a value of $m = 4$ was used in order to compare with referenced results to insure the rapid convergence of the series, and to note the effect of a change in m.

The program was checked out by comparison with published results. The phase shifts and coefficients of the Legendre series for the Coulomb scattering amplitude (Table I and II respectively of Ref. [3]) were reproduced with good accuracy. Also, cross sections for scattering from Carbon-12 at an incident electron energy of 60 Mev, obtained from Yale University, were matched with good agreement The Yale results were obtained using the same program with $m = 3$.

All of the calculations are done in the center-of-mass system. The laboratory input parameters are converted to this system by the formulas generated using the well-known transformation laws provided by the special theory of relativity. The equations used are contained in reference [11].

III. RESULTS

The results for various conditions in the electron-nucleus scattering process are contained in Tables I - VI. All cross sections are given in f^2. Tables I - IV contain the phase shift cross section and a quantity called "Phase Shift Formfactor Squared", which is the ratio of the phase shift cross section to the Mott point nucleus cross section. Tables V and VI contain the phase shift cross section, the "Phase Shift Formfactor Squared", and a quantity called "Born Formfactor Squared". The "Born Formfactor Squared" is the ratio of the Born approximation cross section to the Mott cross section. The incident electron energies used are 10 - 100 MeV for Tables I - IV and 10 - 150 MeV for Tables V and VI. All results are given for scattered electron angles of 45°, 90°, and 135°.

The Born form factor is a derived quantity and is related to the Fourier transform of the charge distribution. A plot of the Born form factor versus the transferred momentum from the electron to the nucleus yields the radius of the nucleus by the slope of the plot near the origin. The "Phase Shift Formfactor" does not have such a simple interpretation.

The results in Table I are for the Carbon-12 nucleus. The charge distribution used is the gaussian p-shell model, mentioned earlier in Section II. The parameter values used are $a = 1.648f$ and $\alpha = 1.056$.

The results in Table II are for the same conditions as Table I with the exception that the value of the parameter, a, was changed to give a 10% increase in the rms radius of Carbon-12. This new value is $a = 1.813f$. The value of α was not changed.

From the results, this change in the value of the parameter, a, produced a percentage change in the phase shift cross section ranging from 0.06% at 10 MeV to 6% at 100 MeV, for a scattering angle of 45°.

Table III contains results for scattering from the Lithium-6 nucleus. The charge distribution used is the empirical form developed by Suelzle, and was also mentioned earlier in Section II. The parametric values used were $a^2 = 0.87f$, $b^2 = 1.70f$, and $c^2 = 0.205f$.

The results of Table IV are for the same conditions as Table III with the exception that the value of the parameter, a, was changed to give a 10% increase in the rms radius of Lithium-6. The new value is $a^2 = 1.195f^2$. Approximately the same percentage change in the phase shift cross section was observed here as for Carbon-12.

Tables V and VI contain results for the same conditions as Tables I and III, with the addition of the quantity Born Formfactor Squared. The expressions used for the calculations of the Born Formfactor are:

For Carbon-12, from reference [13]

$$F(q^2) = [1 - \alpha a^2 q^2/2(2 + 3\alpha)] \exp (- \tfrac{1}{4} q^2 a^2)$$

where a and α are the same parameters used in Table I and q is the momentum transfer.

For Lithium-6, from reference [7]

$$F(q^2) = \exp(- a^2 q^2) - c^2 q^2 \exp(- b^2 q^2)$$

where a^2, b^2, and c^2 are the same parameters used in Table III.

While the same parameters for the given charge distribution were used in Tables V and VI, as compared to I and II, there was a change made in the value of the fitting radius used for the two cases. In the numerical integration routine used, integration is from the origin out to x_0, where, as was mentioned earlier, $x_0 = r_0 k$. Since k is a function of the momentum, and hence the incident energy of the electron, an increase in the energy will cause an increase in the value of x_0. The step size, or spacing between points where step-by-step integration is done, is a fixed parameter. Thus, for given storage space in the computer, there exists an energy at

which all storage will be utilized prior to reaching x_o in the integration process. For high energies, this problem can be alleviated by lowering the value of r_o, the fitting radius in fermi's.

To circumvent this storage problem inherent in using energies above 100 MeV, a fitting radius value of 8.0f was used for all calculations in Tables V and VI, compared to a value of 10.0 used for calculations in Tables I, II, III, and IV. The effect of this change in fitting radius value can be seen by comparison of the phase shift cross section results between Tables I and V, or between Tables III and VI. Also shown in Figure 1, is a plot of the difference between the "Phase Shift Formfactor Squared" and the "Born Formfactor Squared", labeled as $F_p^2 - F_b^2$, as a function of incident electron energy.

IV CONCLUSIONS

The "exact" phase shift analysis provides a means for comparison of theoretical results with experimental data. To uniquely find a charge distribution which fits all experimental data requires more calculations than are given here. The value of the phase-shift analysis lies in its applicability to any scattering situation, being restricted only by the numerical methods used. Many more charge distributions could, and should, be used to compare results with those given here.

A comparison of the results obtained using the phase shift analysis and the Born approximation can be made from the values of "Phase Shift Formfactor Squared" and "Born Formfactor Squared", since both of the quantities represent the respective cross-sections divided by the Mott cross-section. Agreement between these results is good at small angle scattering for all energies considered. Deviation between the two occurs for large angle scattering at energies above 150 Mev. While the exact cause for this deviation is not known, it is believed to be due to particular numerical techniques used.

TABLE I

Carbon-12
Incident electron energy = E

Angle in degrees	Phase Shift Cross Section, f^2	Phase Shift Formfactor Squared
E = 10 MeV		
45	7.6990	1.0311
90	0.39459	1.0500
135	0.040232	1.0526
E = 20 MeV		
45	1.9077	1.0264
90	0.094976	1.0176
135	0.0093839	0.99842
E = 30 MeV		
45	0.83991	1.0181
90	0.040004	0.96652
135	0 0037821	0.90963
E = 40 MeV		
45	0.46169	0.99538
90	0.020885	0.89814
135	0.0018695	0 80133
E = 50 MeV		
45	0.28845	0.97210
90	0.012170	0.81867
135	0.0010046	0.67421
E = 60 MeV		
45	0.19151	0.92960
90	0.0074793	0.72516
135	0.00056986	0.55164
E = 70 MeV		
45	0.13570	0.89680
90	0.0047274	0.62444
135	0.00032788	0.43274
E = 80 MeV		
45	0.099369	0.85799
90	0.0030472	0.52621
135	0.00018908	0.32648
E = 90 MeV		
45	0.074077	0.80976
90	0.0019975	0.43698
135	0.00011137	0.24378

TABLE I (continued)

Carbon-12
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section, f^2	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.056797	0.76673
90	0.0013337	0.36055
135	0.000067867	0.18369

TABLE II

Carbon-12
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10 MeV		
45	7.6939	1.0304
90	0.39370	1.0476
135	0.040076	1.0485
E = 20 MeV		
45	1.9026	1.0237
90	0.094112	1.0083
135	0.0092373	0.98283
E = 30 MeV		
45	0.83500	1.0121
90	0.039188	0.94680
135	0.0036472	0.87718
E = 40 MeV		
45	0.45704	0.98535
90	0.020134	0.86588
135	0.0017494	0.74985
E = 50 MeV		
45	0.28373	0.95619
90	0.011522	0.77506
135	0.00091793	0.61602
E = 60 MeV		
45	0.18706	0.90802
90	0.0068797	0.66879
135	0.00049508	0.47925
E = 70 MeV		
45	0.13150	0.86904
90	0.0042364	0.55958
135	0.00027068	0.35724
E = 80 MeV		
45	0.095369	0.82345
90	0.0026531	0.45503
135	0.00014646	0.25289
E = 90 MeV		
45	0.070329	0.76879
90	0.0016602	0.36318
135	0.000080749	0.17675

TABLE II (continued)

Carbon-12
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.053271	0.71914
90	0.0010604	0.28665
135	0.000045816	0.12401

TABLE III

Lithium-6
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10MeV		
45	1.9056	1.0206
90	0.095426	1.0161
135	0.0097114	1.0172
E = 20 MeV		
45	0.46574	1.0027
90	0.022975	0.98622
135	0.0022619	0.96539
E = 30 MeV		
45	0.20439	0.99158
90	0.0086254	0.93253
135	0.00090224	0.87180
E = 40 MeV		
45	0.10904	0.94119
90	0.0050287	0.86796
135	0.00044621	0.76960
E = 50 MeV		
45	0.070536	0.95198
90	0.0029227	0.78985
135	0.00023978	0.64855
E = 60 MeV		
45	0.046945	0.91286
90	0.0017908	0.69819
135	0.00012923	0.50501
E = 70 MeV		
45	0.033412	0.88483
90	0.0011178	0.59428
135	0.000076337	0.40736
E = 80 MeV		
45	0.024142	0.83549
90	0.00071629	0.49826
135	0.000044432	0.31067
E = 90 MeV		
45	0.018222	0.79849
90	0.00047169	0.41600
135	0.000028127	0.24969

TABLE III (continued)

Lithium-6
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 100 MeV		
45	0.013743	0.74393
90	0.00031767	0.34651
135	0.000018638	0.20491

TABLE IV

Lithium-6
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared
E = 10 MeV		
45	1.9037	1.0196
90	0.095103	1.0126
135	0.0096554	1.0114
E = 20 MeV		
45	0.46391	0.99872
90	0.022665	0.97290
135	0.0022094	0.94300
E = 30 MeV		
45	0.20261	0.98296
90	0.0093330	0.90420
135	0.00085429	0.82547
E = 40 MeV		
45	0.10728	0.92593
90	0.0047658	0.82259
135	0.00040810	0.70388
E = 50 MeV		
45	0.068858	0.92933
90	0.0026828	0.72501
135	0.0020581	0.55667
E = 60 MeV		
45	0.045327	0.88140
90	0.0015750	0.61405
135	0.00010631	0141544
E = 70 MeV		
45	0.031853	0.84354
90	0.00094298	0.50132
135	0.000056556	0.30180
E = 80 MeV		
45	0.022675	0.78470
90	0.00057131	0.39741
135	0.000029902	0.20907
E = 90 MeV		
45	0.016833	0.73763
90	0.00035251	0.31089
135	0.000017085	0.15167
E = 100 MeV		
45	0.012450	0.67394
90	0.00022082	0.24087
135	0.000010435	0.11473

TABLE V

Carbon-12
Incident electron energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 10 MeV			
45	7.6990	1.0311	0.99713
90	0.39459	1.0500	0.99023
135	0.040231	1.0525	0.98344
E = 20 MeV			
45	1.9073	1.0262	0.98854
90	0.094906	1.0168	0.96153
135	0.0093720	0.99715	0.93527
E = 30 MeV			
45	0.83967	1.83967	0.97444
90	0.039964	0.96554	0.91544
135	0.0037755	0.90803	0.86007
E = 40 MeV			
45	0.46130	0.99455	0.95501
90	0.020922	0.89544	0.85460
135	0.0018594	0.79700	0.76472
E = 50 MeV			
45	0.28774	0.96971	0.93958
90	0.012161	0.81806	0.78205
135	0.0010189	0.68378	0.65708
E = 60 MeV			
45	0.19110	0.92761	0.90156
90	0.007195	0.72906	0.70152
135	0.00057588	0.55747	0.54537
E = 70 MeV			
45	0.13546	0.89522	0.86835
90	0.0047951	0.63338	0.61663
135	0.00032714	0.43176	0.43680
E = 80 MeV			
45	0.099336	0.85770	0.83149
90	0.0031078	0.53666	0.53104
135	0.00018924	0.32675	0.33726
E = 90 MeV			
45	0.074312	0.81233	0.79159
90	0.0020247	0.44292	0.44767
135	0.00010737	0.23501	0.25062

TABLE V (continued)

Carbon-12
Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 100 MeV			
45	0.057197	0.77214	0.74914
90	0.0013247	0.35812	0.36938
135	0.000060509	0.16378	0.17892
E = 150 MeV			
45	0.017031	0.51795	0.51978
90	0.00015640	0.095549	0.09931
135	0.0000022275	0.013672	0.01574

TABLE VI

Lithium-6
Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 10 MeV			
45	1.9056	1.0206	0.99679
90	0.095424	1.0160	0.98908
135	0.0097111	1.0172	0.98146
E = 20 MeV			
45	0.46560	1.0024	0.98719
90	0.022952	0.98521	0.95712
135	0.0022579	0.96370	0.92817
E = 30 MeV			
45	0.20424	0.99083	0.97138
90	0.0095998	0.93005	0.90645
135	0.00089803	0.86773	0.84682
E = 40 MeV			
45	0.10880	0.93908	0.94985
90	0.0050181	0.86614	0.84075
135	0.00044916	0.77469	0.74646
E = 50 MeV			
45	0.070242	0.04801	0.92291
90	0.0029116	0.78685	0.76421
135	0.00024328	0.65802	0.63964
E = 60 MeV			
45	0.046778	0.90962	0.89118
90	0.0017999	0.70170	0.68125
135	0.00013537	0.52899	0.52724
E = 70 MeV			
45	0.03328	0.88262	0.85527
90	0.0011456	0.60903	0.59617
135	0.000078033	0.41641	0.42424
E = 80 MeV			
45	0.024143	0.83550	0.81587
90	0.00074133	0.51568	0.51267
135	0.000044886	0.31384	0.33253
E = 90 MeV			
45	0.018326	0.80308	0.77375
90	0.00048518	0.42790	0.43357
135	0.000026574	0.23590	0.25431

TABLE VI (continued)

Lithium-6
Incident Electron Energy = E

Angle in Degrees	Phase Shift Cross Section	Phase Shift Formfactor Squared	Born Formfactor Squared
E = 100 MeV			
45	0.013904	0.75263	0.72951
90	0.00031586	0.34454	0.36096
135	0.000015852	0.17429	0.19003
E = 150 MeV			
45	0.0039987	0.48824	0.50086
90	0.000049157	0.12171	0.11665
135	0.0000012616	0.031705	0.031708

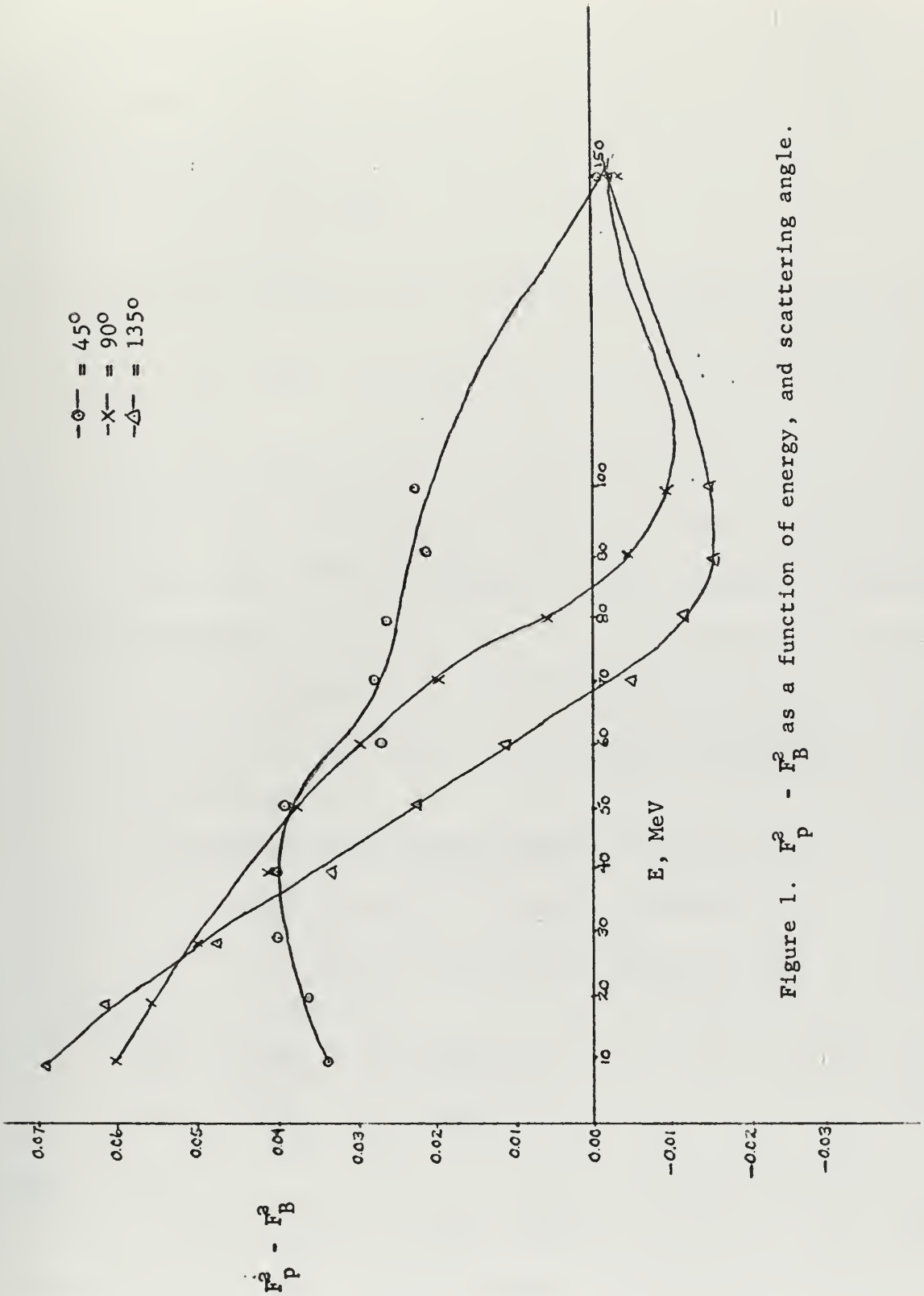

Figure 1. $F_p^2 - F_B^2$ as a function of energy, and scattering angle.

APPENDIX A

The notations and method of calculation used are those of Rawitscher [4], and are shown here for convenience:

The following notation is used,

E = total energy/mc^2

p = momentum/mc

$\alpha = Ze^2/\hbar c$

$\beta = v/c = p/E$

$\gamma = \alpha/\beta$

$\gamma' = (1 - \beta^2)^{\frac{1}{2}}$

$s_k = + (k^2 - \alpha^2)^{\frac{1}{2}}$ for regular solutions, denoted by superscript R,

$s_k = - (k^2 - \alpha^2)^{\frac{1}{2}}$ for irregular solutions, denoted by superscript I,

$\mathcal{K} = mcp/\hbar$

r = radial distance from center of nucleus

$x = r\mathcal{K}$, $x_o = r_o\mathcal{K}$, where r_o is the matching of fitting-on radius

$mc^2 = 0.511$ MeV

k = angluar momentum quantum number $\pm 1, \pm 2, \ldots\ldots$

The radial wave functions $F_k(x)$ and $G_k(x)$, defined by

$$G_k = r^{-1}(E + 1)^{\frac{1}{2}} g_k, \quad F_k = r^{-1}(E - 1)^{\frac{1}{2}} f_k \tag{1a}$$

obey the radial equations

$$\begin{aligned} (d/dx - k/x)g_k + (1 - v_1)f_k &= 0 \\ (d/dx + k/x)f_k - (1 - v_2)g_k &= 0 \end{aligned} \tag{2a}$$

where

$$v_1 = \Phi(E - 1)/p^2, \; v_2 = \Phi(E + 1)/p^2, \tag{3a}$$

and where Φ is the Coulomb potential energy in units of mc^2. For the example of a point nucleus, $\Phi/p = - \alpha/x$.

The phase shifts η_k are defined in the usual manner [5] by the

asymptotic form of the radial wave functions of Eq. (1a):

$$\begin{aligned} G_k &\approx r^{-1} \sin [x - (k - 1)\,\pi/2 + \eta_k], \quad k > 0 \\ &\approx r^{-1} \sin [x - |k|\,\pi/2 + \eta_k], \quad k < 0 \end{aligned} \tag{4a}$$

The value of η_k is obtained in terms of the regular and irregular Coulomb phase shifts η_k^R, η_k^I and the matching coefficients $(D/C)_k$ from

$$\tan \eta_k = \frac{\sin \eta_k^R + (D/C)_k \sin \eta_k^I}{\cos \eta_k^R + (D/C)_k \cos \eta_k^I} \tag{5a}$$

The Coulomb phase shifts are given by

$$\eta_k^{R,\,I} = (X + Y)_k^{R,I} \tag{6a}$$

$$\begin{aligned} X_k &= (k - 1 - s_k)\,\pi/2 - \arg \Gamma(s_k + 1 + i\gamma), \quad k > 0 \\ X_k &= X_{|k|} + \pi/2 \qquad\qquad\qquad\qquad k < 0 \end{aligned} \tag{7a}$$

For the sake of clarity the superscripts R and I have been omitted in the above equation. The value of the argument of Γ is calculated by means of Stirling's approximation [12]. The value of Y is given in expression below, valid for both signs of k:

$$\begin{aligned} \sin Y_k &= -k[k\,(k + s_k) + \gamma'\,(\gamma' - \gamma)]^{\frac{1}{2}} / \left(|k|\;|k - i\gamma'|\;2^{\frac{1}{2}}\right) \\ \cos Y_k &= [k\,(k - s_k) + \gamma'\,(\gamma' + \gamma)]^{\frac{1}{2}} / \left(|k - i\gamma'|\;2^{\frac{1}{2}}\right) \end{aligned} \tag{8a}$$

The matching coefficients $(D/C)_k$ are obtained in terms of the radial wave functions evaluated at x_o:

$$(D/C)_k = \left[\frac{g'^R - f'^R(g/f)}{(g/f)f'^I - g'^I}\right]_k (N^R/N^I)_k x_o^{\,2|s_k|} \tag{9a}$$

Here g and f are the solutions of Eqs. (2a) and the primed quantities are related to the point Coulomb radial waves $G^{R,I}$, $F^{R,I}$ by means of

$$\begin{aligned} G_k^{R,I} &= r^{-1} N_k^{R,I}\, x_o^{s_k}\, g_k'^{R,I} \\ F_k^{R,I} &= r^{-1}[(E - 1)/(E + 1)]^{\frac{1}{2}}\, N_k^{R,I}\, x_o^{s_k}\, f_k'^{R,I} \end{aligned} \tag{10a}$$

The g' and f' are given by the series expansion [3]

$$g' = \sum a_m x_o^m, \qquad f' = \sum b_m x_o^m \tag{11a}$$

$$\begin{aligned} a_m &= [-(\gamma - \gamma')a_{m-1} - (s_k + m + k)b_{m-1}]/[m(m + 2s_k)], \\ b_m &= [(s_k + m - k)a_{m-1} - (\gamma + \gamma')b_{m-1}]/[m(m + 2s_k)], \\ b_o &= (\gamma + \gamma')/(k + s_k), \; a_o = 1 \end{aligned} \tag{12a}$$

In Eq. (12a) the superscripts R and I and the subscripts k have been omitted for the sake of clarity.

The normalization coefficients N are obtained by comparing the G and F of Eq. (10a) with those given in terms of the hypergeometric functions [5],

$$N_k^{R,I} = -(k/|k|)2^{s_k} e^{\pi\gamma/2} \left[\frac{k(k + s_k) + \gamma'(\gamma' - \gamma)}{2(k^2 + \gamma')}\right]^{\frac{1}{2}} \cdot$$

$$|\Gamma(s_k + 1 + i\gamma)|/[\Gamma(2s_k + 1)]. \tag{13a}$$

The ratio $(N^R/N^I)_k$ is most convenient in the form

$$(N^R/N^I)_k = \frac{|\Gamma(\rho_k + i\gamma)|^2}{|\Gamma(2\rho_k)|^2} \frac{(\rho_k^2 + \gamma^2)^{\frac{1}{2}}}{2\rho_k} \cdot \frac{X[\cos h^2(\pi\gamma) - \cos^2\pi\rho_k]^{\frac{1}{2}}}{\sin 2\pi\rho_k} \tag{14a}$$

$$X 2^{2\rho k}\left\{[k(k + \rho_k) + \gamma'(\gamma' - \gamma)]/[k(k - \rho_k) + \gamma'(\gamma' - \gamma)]\right\}^{\frac{1}{2}}$$

$$\rho_k = |s_k|.$$

Finally, the scatterin amplitudes [5] f(θ) and g(θ), from which the cross section 6(θ) is obtained, are given in terms of the Legendre polynomials $P_k(\cos\theta)$ as

$$\begin{aligned} f(\theta) &= (2ik)^{-1} \sum_k c_k P_k \\ g(\theta) &= (2ik\sin\theta)^{-1} \sum_k d_k P_k \\ c_k &= (2k + 1)(e^{i\eta_{k+1}} - 1) + k\alpha_k \end{aligned} \tag{15a}$$

$$d_k = [(k + 1)(k + 2)\alpha_{k+1}/(2k + 3)] - k(k - 1)\alpha_{k-1}/(2k - 1) \qquad (16a)$$

$$\alpha_k = e^{2i\eta} - |k| - e^{2i\eta_{k+1}}$$

$$\sigma(\theta) = |f(\theta)|^2 + |g(\theta)|^2$$

```
C                                                                       1B000
C     THIS PROGRAM IS USED TO CALCULATE SCATTERING CROSS SECTIONS       2B000
C     FOR ELECTRONS INCIDENT ON NUCLEI. THE METHODS USED ARE            3B000
C     BASICALLY THOSE OF RAWITSCHER AND CAN BE FOUND IN VOLUME 112      4B000
C     NUMBER 4,PHYSICAL REVIEW,PAGE 1274. WHILE THERE IS MUCH           5B000
C     DESCRIPTIVE COMMENT CONTAINED IN THIS PROGRAM,AN EVEN MORE        6B000
C     DETAILED EXPLANATION OF THE METHODS USED CAN BE OBTAINED FROM     7B000
C     PROFESSOR F. BUSKIRK,PHYSICS DEPARTMENT,NPS.                      8B000
C                                                                       9B000
C     MOST OF THE COMMENTS CONTAINED HEREIN WILL PERTAIN TO ACTUAL     10B000
C     USAGE OF THE PROGRAM,ESPECIALLY IN REGARD TO ITS MECHANICAL      11B000
C     LIMITATIONS AND CAPABILITIES. A DETAILED SET OF COMMENTS IS      12B000
C     PRESENT IN THE YALERF SUBPROGRAM DUE TO THE COMPLEXITY OF        13B000
C     THE PROGRAM.                                                     14B000
C                                                                      14B000
C     ALL THE COMMENTS CONTAINED IN THE PROGRAM PERTAIN TO THE         15B000
C     STEP OR SET OF STEPS IMMEDIATELY PRECEDING THEM.                 16B000
C                                                                      17B000
C                                                                       1A003
C     THIS IS THE MAIN CONTROL PROGRAM FOR YALERF. IT CONTROLS THE      2A003
C     INPUT AND OUTPUT. THE PROGRAM HAS 11 INPUT PARAMETERS WHICH ARE   3A003
C     CONTAINED ON 2 CARDS. THESE PARAMETERS,WITH FORMAT AND UNITS ARE  4A003
C     AS FOLLOWS:                                                       5A003
C     SYMBOL   DESCRIPTION                        FORMAT      UNITS     6A003
C     CARD 1                                                            7A003
C     Z        NUCLEAR CHARGE                     F10.5       DIMENSIONLESS  8A003
C     A        ATOMIC WEIGHT                      F10.5       DIMENSIONLESS  9A003
C     P1       1ST PARAMETER                      F10.5       SEE BELOW  10A003
C     P2       2ND PARAMETER                      F10.5       SEE BELOW  11A003
C     P3       3RD PARAMETER                      F10.5       SEE BELOW  12A003
C     MODEL    CHARGE DISTRIBUTION                I10         DIMENSIONLESS  13A003
C              SELECTOR                                                 14A003
C     CARD 2                                                            15A003
C     EO       INCIDENT ELECTRON ENERGY           F10.5       MEV        16A003
C     TI       INITIAL ANGLE                      F10.5       DEG        17A003
C     T2       FINAL ANGLE                        F10.5       DEG        18A003
C     TH       ANGLE STEP                         F10.5       DEG        19A003
C     RO       FITTING ON RADIUS                  F10.5       FM         20A003
C                                                                       21A003
C     EXPLANATION OF PARAMETERS:                                        22A003
C     VARIABLE       CHARGE DISTRIBUTION TYPE                           23A003
C                    FERMI        GAUSSIAN(P-SHELL)                     24A003
C     MODEL          1            2                                     25A003
C     P1             C(FM)        A(FM)                                 26A003
C     P2             T(FM)        ALPHA                                 27A003
C     P3             -            -                                     28A003
C                                                                       29A003
C     THE PROGRAM CAN CONTAIN HAS MANY DIFFERENT CHARGE DISTRIBUTIONS   30A003
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C     AS ARE DESIRED. IT PRESENTLY CONTAINS 5,BUT ONLY THE FIRST 2      31A003
CCC   INDICATED ABOVE CAN HAVE THEIR PARAMETERS CONTROLLED BY INPUT,     32A003
CCC   ALTHOUGH THIS COULD BE CHANGED.                                    33A003
CCC                                                                      34A003
CCC   FERMI      P(R)=1/(1+EXP(R-C/(T/4.4)))                             35A003
CCC                                                                      36A003
CCC   GAUSSIAN                                                           37A003
CCC   P-SHELL    P(R)=(1+ALPHA(R/A)**2)*EXP(-(R/A)**2)                   38A003
CCC                                                                      39A003
CCC   MODEL NUMBERS 3-5 SELECT OTHER CHARGE DISTRIBUTIONS THAT ARE       40A003
CCC   INDICATED IN FMOD SUBPROGRAM. TO CHANGE ANY OF THE PARAMETERS      41A003
CCC   OF THE MODELS, IT IS NECESSARY TO CHANGE PROGRAM STEP.              42A003
CCC                                                                      43A003
CCC   TO USE PROGRAM,FIRST CARD IN DATA DECK SHOULD BE AS PER CARD 1     44A003
CCC   ABOVE. EACH DIFFERENT ENERGY INPUT,FOR SAME CARD 1 PARAMETERS,     45A003
CCC   REQUIRES A SEPARATE CARD OF CARD 2 TYPE. PLACE AS MANY AS NEEDED   46A003
CCC   BEHIND CARD 1. AT PRESENT,THE PROGRAM CAN CALCULATE CROSS SECTIONS47A003
CCC   FOR UP TO 100 DIFFERENT ENERGIES FOR EACH NUCLEUS. TO TERMINATE    48A003
CCC   PROGRAM,OR TO CHANGE TO NEW CARD 1 DATA,PLACE A BLANK CARD AFTER   49A003
CCC   LAST CARD OF CARD 2 TYPE. THIS BLANK CARD CAUSES IF STATEMENT ON   50A003
CCC   CARD SEQUENCE #014 TO TRANSFER TO INITIAL READ STATEMENT. THE NEW  51A003
CCC   CARD 1 TYPE IS FOLLOWED BY ITS SET OF ENERGY CARDS. IF NO MORE     52A003
CCC   CALCULATIONS ARE DESIRED, PLACE 0.0 IN Z FORMAT OF NEW CARD 1.     53A003
CCC                                                                      54A003
CCC   IN REGARDS TO PRINTED OUTPUT,SIGMA=SCATTERING CROSS SECTION,       55A003
CCC   SIGMA(MOTT)=POINT NUCLEUS CROSS SECTION FOR GIVEN INPUT DATA,      56A003
CCC   AND FORMFACTOR IS RATIO OF SIGMA/SIGMA(MOTT). THE UNITS OF OUTPUT  57A003
CCC   CROSS SECTIONS ARE SQUARE FERMI'S.                                 58A003
CCC   IT SHOULD BE NOTED THAT IF A MODEL NUMBER OTHER THAN 1 OR 2 IS      59A003
CCC   USED,THEN P1,P2,AND P3 SHOULD BE PUT=0,AS THEY ARE ON PRINTED      60A003
CCC   OUTPUT AND ARE NOT APPLICABLE TO MODELS OTHER THAN 1 OR 2.         61A003
CCC                                                                      62A003
CCC   THE QUANTITIES T1,T2,AND TH ARE PRESENTLY SET TO COINCIDE WITH     63A003
CCC   SCATTERING PORTS OF THE NPS LINAC; 45-135 DEGREES IN 15 DEGREE     64A003
CCC   STEPS.                                                             65A003
CCC                                                                      66A003
CCC   THE FITTING RADIUS RO PERTAINS TO THE MATCHING OF NUCLEAR AND      67A003
CCC   COULOMB WAVE FUNCTIONS AND IS DISCUSSED IN RAWITSCHER'S ARTICLE.   68A003
CCC   IT HAS BEEN FOUND THAT A RUN FOR CARBON,WITH 20 DIFFERENT          69A003
CCC   INCIDENT ENERGIES REQUIRES APPROXIMATELY ONE MINUTE OF COMPUTER     70A003
CCC   TIME.                                                              71A003
CCC                                                                      72A003
CCC   THE EXISTING PROGRAM CARDS ALL HAVE SEQUENCE NUMBERS ON THEM.      73A003
CCC   IF AN OTHER THAN PERMANENT CHANGE IS MADE TO PROGRAM,IT IS          74A003
CCC   RECOMMENDED THAT A DIFFERENT SEQUENCE NUMBERING SYSTEM BE USED     75A003
CCC   TO FACILITATE KEEPING TRACK OF CHANGES.                            76A003
C                                                                        77A003
      DIMENSION THEXX(100),SIGTXX(100),SIGMTX(100),FELSXX(100)
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```
      DIMENSION              SIGMTC(100),RATIO(100),SIGCM(100),THCM(100)      000
      COMMON S(950),S1(950),SLOC(950)                                         001
      COMMON SLOC1(950)                                                       002
      COMMON EPHI(950),EPP(950),EPPP(950)                                     003
C
    1 READ(5,9000)Z,A,P1,P2,P3,MODEL                                          007
 9000 FORMAT(5F10.5,I10)                                                      008
      IF(Z)2,999,2                                                            009
    2 CONTINUE                                                                010
      DO10J=1,100                                                             011
      READ(5,9010)E0,T1,T2,TH,R0                                              012
 9010 FORMAT(5F10.5)                                                          013
      IF(E0)3,1,3                                                             014
    3 CONTINUE                                                                015
      WRITE(6,9020) Z,A,MODEL,P1,P2,P3,E0,R0                                  016
 9020 FORMAT(28H1ELASTIC ELECTRON SCATTERING /14H CROSS SECTION//             017
     14H Z =,F10.5/4H A =,F10.5/4H M =,I10/4H P1=,F10.5/4H P2=,F10.5/         018
     24H P3=,F10.5//4H E0=,F10.5///4H R0=,F10.5///)                           019
      WRITE(6,9030)                                                           020
 9030 FORMAT(T6,'THETA',T19,'SIGMA',T32,'SIGMA(MOTT)',T49,'FORMFACTOR')       021
      T=T1                                                                    022
      DO40L=1,100                                                             023
C                                                                        1A023
CC    THIS INDICATES THAT UP TO 100 ANGLE STEPS MAY BE USED IF DESIRED.  2A023
C                                                                        3A023
      THEXX(L)=T                                                              024
      IF(T-T2)50,30,30                                                        025
   50 T=T+TH                                                                  026
   40 CONTINUE                                                                027
   30 JMAX=L                                                                  028
C                                                                        1A028
CC    JMAX IS EQUAL TO THE NUMBER OF SCATTERING ANGLES THAT CALCULATIONS  2A028
CC    WILL BE DONE FOR.                                                  3A028
C                                                                        4A028
      CALL SIGTRU(E0,ECM,THEXX,THCM,JMAX,A,Z,MODEL,P1,P2,P3,R0,SIGTXX,        029
     1SIGCM,SIGMTX,SIGMTC,FELSXX,RATIO)                                       030
C                                                                        1A030
CC    THE SUBPROGRAM SIGTRU IS CALLED AND ALL PARAMETERS TRANSFERRED      2A030
CC    TO IT ARE INDICATED. THE VARIABLE AND ARRAY NAMES USED IN SIGTRU    3A030
CC    FOR THESE PARAMETERS ARE NOT NECESSARILY THE SAME. THIS WAS DONE    4A030
CC    TO PROVIDE CLARITY WHILE FORMING COMPLETE PROGRAM. WHEREVER         5A030
CC    POSSIBLE,VARIABLE AND ARRAY NAMES ARE USED WHICH ABBREVIATE         6A030
CC    ACTUAL QUANTITY IN THEORETICAL WORK.                                7A030
C                                                                        8A030
      DO20L=1,JMAX                                                            031
   20 WRITE(6,9040)THEXX(L),SIGTXX(L),SIGMTX(L),FELSXX(L)                     032
 9040 FORMAT(F10.5,3E16.5)                                                    033
   10 CONTINUE                                                                034
```

```
  999 STOP                                                                035
      END                                                                 036

      SUBROUTINE SIGTRU(E1,E1CM,TL,TCM,JM,AM,Z,MOD,C,T,W,FITRAD,SIGLAB, SIG00010
     1SIGCM,SIGMTL,SIGMTC,FELS,RATIO)                                    SIG00020
      DIMENSION TL(100),TCM(100),RATIO(100),SM(100),FELS(100),           SIG00030
     1SIGLAB(100),SIGCM(100),SIGMTL(100),SIGMTC(100)                     SIG00040
C                                                                          1AS40
CCC   THIS IS THE SUBPROGRAM USED FOR THE TRANSFORMATION FROM CENTER       2AS40
CCC   OF MASS COORDINATE SYSTEM,IN WHICH CALCULATIONS ARE DONE, TO         3AS40
CCC   LAB SYSTEM OF COORDINATES. THIS TRANSFORMATION IS DONE ACCORDING     4AS40
CCC   TO THE RELATIONS IN THE ARTICLE BY DEDRICK, REVIEWS OF MODERN        5AS40
CCC   PHYSICS, VOLUME 34,NUMBER 3,PAGE 429.                               6AS40
CC                                                                         7AS40
      EM2=AM*931.478                                                   SIG00080
      EM1=.51106                                                       SIG00090
      ETCM=SQRT(EM1**2+EM2**2+2.*E1*EM2)                               SIG00100
      E1CM=(ETCM**2+EM1**2-EM2**2)/(2.0*ETCM)                          SIG00110
C                                                                          1AS110
CCC   E1CM IS THE INCIDENT ENERGY OF ELECTRON IN CM FRAME.                 2AS110
CC                                                                         3AS110
      A=(E1+EM1**2/EM2)/(E1+EM2)                                       SIG00120
      G=(E1+EM2)/ETCM                                                  SIG00130
      CK=1.0-A*A                                                       SIG00140
      DO 40 I=1,JM                                                     SIG00150
C                                                                          0AS150
CCC   SINCE JM=JMAX IN PHASE,WE CALCULATE ANGLE IN CM FRAME FOR EACH       1AS150
CCC   ANGLE IN LAB FRAME FOR WHICH RESULTS ARE DESIRED.                    2AS150
CC                                                                         3AS150
      PHI=TL(I)*3.1415926/180.                                         SIG00160
      CS=COS(PHI)                                                      SIG00170
      SN=SIN(PHI)                                                      SIG00180
      AN=CS*SQRT(G*G*CK*SN**2+CS**2)-1.0*A*G*G*SN**2                   SIG00190
      AD=G*G*SN**2+CS**2                                               SIG00200
      COSPH=AN/AD                                                      SIG00210
      THCM=ARCOS(COSPH)                                                SIG00220
      TCM(I)=THCM*180./3.1415926                                       SIG00230
C                                                                          1AS230
CCC   THIS IS ARRAY OF ANGLES IN CM FRAME CORRESPONDING TO GIVEN LAB       2AS230
CCC   FRAME ANGLES.                                                        3AS230
CC                                                                         4AS230
      A1=G*G*CK*SN**2+CS**2                                            SIG00240
      A2=1.0-2.0*CS**2                                                 SIG00250
      TOP=AD*(G*G*CK*A2+2.0*CS**2)                                     SIG00260
      TOP=TOP+2.0*(G*G*A*SQRT(A1)-(1.0-G*G)*A1)*CS                     SIG00270
      BOT=AD**2*SQRT(A1)                                               SIG00280
   40 RATIO(I)=TOP/BOT                                                 SIG00290
```

```
C                                                                       1AS290
CCC     THIS IS THE FACTOR WHICH MULTIPLIES CROSS SECTIONS CALCULATED IN  2AS290
CCC     CM FRAME TO GIVE CROSS SECTIONS IN LAB FRAME.                     3AS290
C                                                                       4AS290
      CALL YALERF(E1CM,TCM,JM,AM,Z,MOD,C,T,W,FITRAD,SIGCM,SIGMTC,FELS)  SIG00300
C                                                                       1AS300
CCCC    THE SUBPROGRAM YALERF IS CALLED AND ALL PARAMETERS TRANSFERRED    2AS300
CCCC    TO IT ARE INDICATED. THE YALERF SUBPROGRAM IS WHERE ALL CROSS     3AS300
CCCC    SECTION CALCULATIONS ARE DONE.                                    4AS300
C                                                                       5AS300
      DO 50 I=1,JM                                                      SIG00310
      SIGMTL(I)=SIGMTC(I)*RATIO(I)                                      SIG00320
      SIGLAB(I)=SIGCM(I)*RATIO(I)                                       SIG00330
      FELS(I)=SIGLAB(I)/SIGMTL(I)                                       SIG00340
   50 CONTINUE                                                          SIG00350
      RETURN                                                            SIG00360
      END                                                               SIG00370

      SUBROUTINE YALERF(EINCX,THEXX,LXXXXX,AXXXX,ZXXXX,MODEL,C,TXXXX,WXXYAL00010
     1XX,FITRAD,SIGTXX,SIGMTX,FELSXX)                                   YAL00020
      COMMON S(1100),S1(1100),SLOC(1100)                                YAL00030
      COMMON SLOC1(1100)                                                YAL00040
      COMMON EPHI(1100), EPP(1100), EPPP(1100)                          YAL00050
      DOUBLE PRECISION  A,FR,GR,FI,GI,SVOFK,ALPHA,ALPHA2,EALP,PUC2      YAL00060
      DOUBLE PRECISION  PUC,     TEMP,BETA,GM,SQB,GP,CK,GGP,PHIK,S      YAL00070
      DOUBLE PRECISION  XO,X1,ZKR,ZKI,ANR1,ANI1,BNR1,BNI1,DOMR,DOMI     YAL00080
      DOUBLE PRECISION  FRNEG,GINEG,FINEG,XFR,XFI,XGR,XGI,T             YAL00090
      DOUBLE PRECISION  ANR,BNR,ANI,BNI,    GRP,FRP,FIP,GIP,GRNEG       YAL00100
      SQS(X,Y)=X**2+Y**2                                                YAL00110
      CSHY(X)=(EXP(X)+EXP(-X))/2.                                       YAL00120
      SSHY(X)=(EXP(X)-EXP(-X))/2.                                       YAL00130
      GAM1(X,Y)=(X-.5)*.5*ALOG(SQS(X,Y))-Y*ATAN(Y/X)-X+.5*ALOG(6.2831   YAL00140
     1185)+X/(12.*SQS(X,Y))-(X**3-3.*Y**2*X)/(360.*SQS(X,Y)**3)         YAL00150
     2+(X**5-10.*X**3*Y**2+5.*X*Y**4)/(1260.*SQS(X,Y)**5)-((X**7-21.*X* YAL00160
     3*5*Y**2+35.*X**3*Y**4-7.*X*Y**6)/(1680.*SQS(X,Y)**7))             YAL00170
      GAM3(X,Y)=.5*((X-.5)*2.*ATAN(Y/X)+Y*ALOG(SQS(X,Y))-2.*Y-Y/(6.*S   YAL00180
     1QS (X,Y))+2.*(3.*X**2*Y-Y**3)/(360.*SQS(X,Y)**3))                 YAL00190
     2-((5.*Y*X**4-10.*Y**3*X**2+Y**5)/(1260.*SQS(X,Y)**5))             YAL00200
     3+((Y*(7.*X**6-35.*X**4*Y**2+21.*X**2*Y**4-Y**6))/(1680.*SQS(X,Y)* YAL00210
     4*7))                                                              YAL00220
      GAM4(X,Y)=-ATAN(Y/X)-ATAN(Y/(X+1.))-ATAN(Y/(X+2.))+GAM3((X+3.     YAL00230
     1),Y)                                                              YAL00240
      DIMENSION Y(3),Y1(3),Y2(3),                                       YAL00250
     1                          AX(4),AA(4),B(4),BA(4),                 YAL00260
     2AM(4),ANM(4),PM(4),ETAKP(140),ETAKN(140),ETKP(140),ETKN(140),COR(1YAL00270
     340,5),COI(140,5),ALR(140),ALI(140),DOR(140,5),                    YAL00280
     4ZP(140),F(600),G(600),DOI(140,5),ATA(140),ETI(140)                YAL00290
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      DIMENSION A(25),FR(600),GR(600),FI(600),GI(600)                    YAL00300
      DIMENSION THEXX(100),SIGTXX(100),SIGMTX(100), FELSXX(100)          YAL00310
C                                                                         1AY310
CC    IN THIS SUBPROGRAM,BEFORE CALCULATIONS CAN BE MADE IT IS NECESSARY  2AY310
CC    TO PUT ALL QUANTITIES IN DIMENSIONLESS FORM APPROPRIATE TO COM-      3AY310
CC    PUTER CALCULATIONS. ALSO,SEVERAL VALUES OF CONSTANTS NEEDED ARE     4AY310
CC    CALCULATED FIRST.                                                   5AY310
C                                                                         6AY310
      EINCX=EINCX-0.5110                                                 YAL00320
C                                                                         1AY320
CC    EINCX=KINETIC ENERGY OF ELECTRON IN CM FRAME.                       2AY320
C                                                                         3AY320
      A(3) = EINCX                                                       YAL00330
6001  A(1) = AXXXX                                                       YAL00340
      A(2) = ZXXXX                                                       YAL00350
      A(4) = 0.511                                                       YAL00360
      A(5) = C/(A(1)**.333333)                                           YAL00370
      A(6) = TXXXX                                                       YAL00380
      A(7) = 0.0                                                         YAL00390
      A(8) = 1.0                                                         YAL00400
      A(9) = 0.7297290-02                                                YAL00410
      A(10) = 0.38615D+03                                                YAL00420
      A(11)=0.156250-01                                                  YAL00430
      A(12) = 0.1953125D-02                                              YAL00440
      A(13) = 0.1D-09                                                    YAL00450
      A(14)= 0.1D-09                                                     YAL00460
      A(15) = 0.0                                                        YAL00470
      A(16) = A(12)                                                      YAL00480
      A(17) = 0.1D-05                                                    YAL00490
      A(18) = 0.                                                         YAL00500
      A(19)=1.0D0                                                        YAL00510
      A(20) = 1.0                                                        YAL00520
      A(21) = 1.0                                                        YAL00530
      A(22) = 0.                                                         YAL00540
      A(23) = 0.                                                         YAL00550
      A(24) = 1.0                                                        YAL00560
C                                                                         1AY560
CC    OF ABOVE VALUES,SOME WERE INITIALLY USED IN TEST RUNS AND IN        2AY560
CC    DEBUGGING PROCEDURES, AND ARE NOT USED IN FINAL PROGRAM.            3AY560
C                                                                         4AY560
      LAG=34                                                             YAL00570
C                                                                         1AY570
CC    LAG VALUE CONTROLS UPPER LIMIT ON SUMMATIONS OVER ANGULAR           2AY570
CC    MOMENTUM QUANTUM NUMBER K(SVOFK IN PROGRAM) CARRIED OUT IN          3AY570
C     LATER CALCULATIONS.                                                 4AY570
C                                                                         5AY570
125   CONTINUE                                                           YAL00580
      SVOFK=1.                                                           YAL00590
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```
C                                                                       1AY590
CCC     THE INITIAL VALUE OF ANGULAR MOMENTUM QUANTUM NUMBER K IS SET   2AY590
CCC     EQUAL TO +1.                                                    3AY590
C                                                                       4AY590
        ALPHA=A(2)*A(9)                                                 YAL00600
C                                                                       1AY600
CCC     THIS IS ALPHA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.      2AY600
C                                                                       3AY600
        ALPHA2=ALPHA**2                                                 YAL00610
        EALP=A(8)*ALPHA                                                 YAL00620
        PUC2=((2.+A(3)/A(4))*A(3))/A(4)                                 YAL00630
        PUC = DSQRT(PUC2)                                               YAL00640
C                                                                       1AY640
CCC     THIS IS MOMENTUM OF INCIDENT ELECTRON IN DIMENSIONLESS UNITS.   2AY640
C                                                                       3AY640
        TEMP=1.+A(3)/A(4)                                               YAL00650
        BETA=PUC/TEMP                                                   YAL00660
C                                                                       1AY660
CCC     THIS IS BETA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.       2AY660
C                                                                       3AY660
        GM=EALP/BETA                                                    YAL00670
C                                                                       1AY670
CCC     THIS IS GAMMA DEFINED IN APPENDIX OF RAWITSCHER'S ARTICLE.      2AY670
C                                                                       3AY670
        SQB=1./TEMP                                                     YAL00680
        GP=GM*SQB                                                       YAL00690
C                                                                       1AY690
CCC     THIS IS PRIMED GAMMA IN APPENDIX OF RAWITSCHER'S ARTICLE.       2AY690
C                                                                       3AY690
        CK=PUC/A(10)                                                    YAL00700
C                                                                       1AY700
CCC     THIS IS KAPPA IN APPENDIX OF RAWITSCHER'S ARTICLE.              2AY700
C                                                                       3AY700
        XO=FITRAD*CK                                                    YAL00740
C                                                                       1AY740
CCC     THIS IS MATCHING RADIUS IN DIMENSIONLESS UNITS. NOTE THAT IF    2AY740
CCC     NEW STEPS ARE PLACED ANYWHERE IN PROGRAM,ALL QUANTITIES WHICH   3AY740
CCC     ARE LINEAR DISTANCES (IN FERMI'S) MUST BE MULTIPLIED BY CK      4AY740
CCC     TO GIVE CORRECT RESULTS.                                        5AY740
C                                                                       6AY740
        LOP=1                                                           YAL00750
C                                                                       1AY750
CCC     THIS IS A RUNNING INDEX WHICH IS USED LATER IN CONJUNCTION WITH 2AY750
CCC     SUMMING OVER ANGULAR MOMENTUM QUANTUM NUMBERS.                  3AY750
C                                                                       4AY750
        CP=C*CK                                                         YAL00760
        Z1P=(A(6)/4.3944)*CK                                            YAL00770
C                                                                       1AY770
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C       THESE ARE 2 CHARGE DISTRIBUTION PARAMETERS IN DIMENSIONLESS UNITS.  2AY770
C                                                                           3AY770
        E1P=(2.+A(3)/A(4))/PUC                                             YAL00780
        EM1P=(A(3)/A(4))/PUC                                               YAL00790
        GGP=ALPHA2/(GM+GP)                                                 YAL00800
C                                                                           1AY800
C       REFER TO NOTES HELD BY PROF. BUSKIRK FOR ABOVE 3 STEPS.             2AY800
C                                                                           3AY800
C                                                                           4AY800
C       WE NOW CALCULATE THE CHARGE DENSITY AND RESULTING POTENTIAL AT      5AY800
C       INCREMENTAL STEPS OUT TO MATCHING RADIUS. THE INTEGRATION IS DONE   6AY800
C       USING SIMPSONS RULE. THE INCREMENTAL STEP VALUES USED ARE THE       7AY800
C       SAME AS THOSE THAT WILL BE USED IN LATER NUMERICAL INTEGRATION      8AY800
C       OF RADIAL WAVE EQUATIONS.                                           9AY800
C                                                                          10AY800
C                                                                          11AY800
   20   RX=0                                                               YAL00840
        M=0                                                                YAL00850
C                                                                           1AY850
C       RX IS THE RADIAL DISTANCE FROM CENTER OF NUCLEUS AND M IS A         2AY850
C       RUNNING INDEX.                                                      3AY850
C                                                                           4AY850
        GRID=A(12)/2.                                                      YAL00860
        XFR=A(12)                                                          YAL00870
        XN=A(12)                                                           YAL00880
C                                                                           1AY880
C       GRID IS A SPACING DISTANCE BETWEEN POINTS WHERE CHARGE DENSITY      2AY880
C       AND DERIVATIVES ARE CALCULATED. XFR AND XN KEEP TRACK OF POINTS     3AY880
C       BETWEEN WHICH SIMPSONS RULE INTEGRATION WAS DONE.                   4AY880
C                                                                           5AY880
        SUM2=0                                                             YAL00890
        SUM3=0                                                             YAL00900
C                                                                           1AY900
C       SUM2 AND SUM3 WILL BE USED TO STORE RESULTS FROM THE 2 INTEGRALS    2AY900
C       NECESSARY TO GET THE POTENIAL V(RX).                                3AY900
C                                                                           4AY900
        DO 25 J=1,1100                                                     YAL00910
        DO23L=1,3                                                          YAL00920
        Y(L)=FMOD(MODEL,RX,CK,C,TXXXX,WXXXX)                               YAL00930
        Y1(L)=Y(L)*RX                                                      YAL00940
        Y2(L)=Y1(L)*RX                                                     YAL00950
   21   RX=RX+GRID                                                         YAL00960
   23   CONTINUE                                                           YAL00970
C                                                                           1AY970
C       THESE STEPS CALCULATE THE VALUE OF THE CHARGE DENSITY AT RX AND     2AY970
C       ALSO RX*(CHARGE DENSITY) AND RX**2*(CHARGE DENSITY). THESE LAST     3AY970
C       2 QUANTITIES ARE THOSE WHICH MUST BE INTEGRATED TO GIVE V(RX).      4AY970
C       THE FUNCTION FMOD IS WHERE THE CHARGE DENSITY CALCULATIONS ARE      5AY970
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C      DONE. THE J=1,3 PROVIDES FOR VALUES AT 3 SUCCEEDING POINTS.          6AY970
C                                                                           7AY970
       RX=RX-GRID                                                          YAL00980
       S(J)=(Y1(1)+4.*Y1(2)+Y1(3))*GRID/3.                                 YAL00990
       S1(J)=(Y2(1)+4.*Y2(2)+Y2(3))*GRID/3.                                YAL01000
       SLOC(J)=Y(3)                                                        YAL01010
       SLOC1(J)=Y2(3)                                                      YAL01020
       M=M+1                                                               YAL01030
C                                                                          1AY1030
CC     THE RESULTS FROM INNER DO LOOP ABOVE ARE USED TO INTEGRATE BY       2AY1030
CC     SIMPSONS RULE. SLOC(J) AND SLOC1(J) ARE USED TO STORE END POINT     3AY1030
CC     OF INTEGRATION VALUES FOR FUTURE USE.                               4AY1030
C                                                                          5AY1030
       IF(J-1098)71,71,22                                                  YAL01040
   71  IF(RX-(XO+A(11)/2.))26,70,70                                        YAL01050
C                                                                          1AY1050
CC     THE 1ST IF STATEMENT IS USED TO ENSURE THAT THE FITTING RADIUS      2AY1050
CC     IS REACHED BEFORE INTEGRATION STOPS DUE TO END VALUE OF DO LOOP.    3AY1050
CC     IT WORKS IN CONJUNCTION WITH 2ND IF STATEMENT WHICH ACTUALLY        4AY1050
CC     CHECKS TO SEE IF XO HAS BEEN REACHED WITHIN A GIVEN INTERVAL.       5AY1050
CC     IF THE FITTING RADIUS HASN'T BEEN REACHED BY J=1098,THEN THE        6AY1050
CC     NEXT RUN THROUGH DO LOOP WILL CAUSE 1ST IF TO TRANSFER TO 22        7AY1050
CC     WHERE THE GRID SPACING IS DOUBLED AND THIS FACT IS PRINTED OUT.     8AY1050
CC     THE ENTIRE SET OF CALCULATIONS IS THEN REPEATED FROM 125 ON.        9AY1050
CC                                                                        10AY1050
CC     NOTE THAT XO IS FUNCTION OF MOMENTUM(DUE TO CK) AND HENCE AS        11AY1050
CC     HIGHER INCIDENT ENERGIES ARE USED, FOR A GIVEN VALUE OF FITRAD,     12AY1050
CC     XO WILL INCREASE, ULTIMATELY CAUSING ABOVE DOUBLING OF SPACING      13AY1050
CC     BETWEEN INTEGRATION STEPS. IF INCIDENT ENERGIES GREATER THAN        14AY1050
CC     APPROXIMATELY 150 MEV ARE USED, THIS WILL OCCUR. TO PREVENT IT,     15AY1050
CC     INCREASE J AND HENCE STORAGE REQUIREMENTS, AND/OR DECREASE FITRAD.  16AY1050
CC                                                                        17AY1050
CC     FOR INFORMATION PURPOSES,AN INCREASE IN J TO 1500 ALONG WITH A      18AY1050
CC     FITRAD=8 FERMI'S WILL ALLOW FOR INTEGRATIONS WITH SAME SPACING      19AY1050
CC     UP TO AN INCIDENT ENERGY OF APPROXIMATELY 250 MEV. THE RESULTS      20AY1050
CC     OBTAINED IF SPACING IS DOUBLED ARE NOT INVALIED BUT CAN'T BE        21AY105
CC     CORRELATED VERY WELL TO LOWER ENERGY RESULTS USING A DIFFERENT      22AY1050
CC     SPACING.                                                            23AY1050
C                                                                          24AY1050
   26  IF(J-1)28,28,300                                                    YAL01060
   28  GRID=A(11)/4.                                                       YAL01070
       XFR=XFR+A(11)/2.                                                    YAL01080
   27  GOTO25                                                              YAL01090
  300  XFR=XFR+A(11)/2.                                                    YAL01100
   25  CONTINUE                                                            YAL01110
C                                                                          1AY1110
CC     A SMALLER SPACING IS USED FOR FIRST INTEGRATION IN ATTEMPT TO       2AY1110
C      GET ACCURATE STARTING POINT. IF(J-1) CAUSES THIS TO BE INCREASED    3AY1110
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C      AND SAME VALUE USED FOR ALL OTHER CALCULATIONS.                          4AY1110
C                                                                               5AY1110
   22  A(11)=A(11)*2.                                                          YAL01120
       WRITE(6,7011)                                                           YAL01130
 7011  FORMAT(85HOSTORAGE CAPACITY HAS BEEN EXCEEDED.GRID IS MULTIPLIED BYAL01140
     1Y 2 AND CALCULATION REPEATED.)                                           YAL01150
       GOTO125                                                                 YAL01160
   70  J=0                                                                     YAL01170
       DO29J=1,M                                                               YAL01180
       SUM2=SUM2+S(J)                                                          YAL01190
       XO=RX                                                                   YAL01200
   29  SUM3=SUM3+S1(J)                                                         YAL01210
C                                                                               1AY1210
C      SUM2 AND SUM3 GIVE TOTAL AREAS UNDER CURVES AFTER COMPLETION OF          2AY1210
C      DO29J=1,M.                                                               3AY1210
C                                                                               4AY1210
       DO501J=2,M                                                              YAL01220
       S1(J)=S1(J)+S1(J-1)                                                     YAL01230
  501  S(J)=S(J)+S(J-1)                                                        YAL01240
C                                                                               1AY1240
C      AFTER COMPLETION OF THIS DO LOOP,EACH S(J) AND S1(J) CONTAINS            2AY1240
C      AREA UNDER CURVE FROM RX=0 TO ITS RELATED RX VALUE.                      3AY1240
C                                                                               4AY1240
       DO30J=1,M                                                               YAL01250
       EPHI(J)=(-EALP/SUM3)*(S1(J)/XN-S(J)+SUM2)                               YAL01260
       EPP(J)=(EALP/XN**2)*(S1(J)/SUM3)                                        YAL01270
       SLOC(J)=SLOC(J)/SUM3                                                    YAL01280
       SLOC1(J)=SLOC1(J)/SUM3                                                  YAL01290
   30  XN=XN+A(11)/2.                                                          YAL01300
C                                                                               1AY1300
C      EPHI(J) IS THE POTENTIAL V(RX) AND EPP(J) IS THE FIRST DERIVATIVE        2AY1300
C      OF THIS POTENTIAL. CERTAIN MANIPULATIONS OF V(RX) FORMULA ARE            3AY1300
C      NECESSARY BEFORE IT HAS ABOVE FORM. REFER TO NOTES HELD BY               4AY1300
C      PROF. BUSKIRK FOR THESE DETAILS.                                         5AY1300
C                                                                               6AY1300
C      NOTE THAT NORMALIZATION CONSTANTS FOR CHARGE DISTRIBUTIONS ARE           7AY1300
C      NOT NEEDED IN USE OF PROGRAM DUE TO DIVISION BY SUM3.                    8AY1300
C                                                                               9AY1300
C                                                                              10AY1300
C      THE CHARGE DENSITIES HAVE BEEN USED TO CALCULATE THE POTENTIAL          11AY1300
C      AND ITS FIRST DERIVATIVE AT LOCATIONS FROM CENTER OF NUCLEUS            12AY1300
C      OUT TO FITTING-ON RADIUS. WITH THIS DATA WE CAN NOW PROCEED TO          13AY1300
C      CALCULATE THE VALUES OF THE REGULAR AND IRREGULAR COULOMB FUNC-         14AY1300
C      TIONS AT THE FITTING-ON OR MATCHING RADIUS.                             15AY1300
C                                                                              16AY1300
C                                                                              17AY1300
   10  PHIK=DSQRT(SVOFK**2-ALPHA2)                                             YAL01340
       ASSIGN 80 TO JACK                                                       YAL01350
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C                                                                       1AY1350
CC      PHIK IS S-SUB-K IN APPENDIX OF RAWITSCHER'S ARTICLE.            2AY1350
C                                                                       3AY1350
   32 T=1.0                                                          YAL01360
      IF(A(16)-A(18))325,325,640                                     YAL01370
  640 IF(A(16)-X0)642,645,645                                        YAL01380
  642 A(16)=A(16)+A(11)                                              YAL01390
      GOTO640                                                        YAL01400
  645 A(16)=A(16)-A(11)                                              YAL01410
  325 X1=A(16)                                                       YAL01420
C                                                                       1AY1420
CC      THE FIRST IF STATEMENT ABOVE IS USED AS A WAY OF LEAVING A(16)  2AY1420
CC      AT ITS INITIAL VALUE. THE SECOND IF STATEMENT COMPARES A(16) WITH 3AY1420
CC      X0. IF A(16) IS LESS THAN X0,AS IT NORMALLY WOULD BE,THEN THE   4AY1420
CC      NEXT SERIES OF STEPS INCREMENT UP UNTIL IT IS A(11) LESS THAN X0. 5AY1420
CC      NOTE THAT AT YAL01200 X0 WAS SET=RX,WHERE RX WAS THEN THE CLOSEST 6DY1420
CC      POINT OF INTEGRATION RESULTS TO ORIGINAL X0. X1 IS SET=THIS FINAL 7AY1420
CC      VALUE OF A(16).                                                 8AY1420
C                                                                       9AY1420
      N=1                                                            YAL01430
      IF(SVOFK)11,12,12                                              YAL01440
   11 ZKR=ALPHA2/(SVOFK-PHIK)                                        YAL01450
      ZKI=SVOFK-PHIK                                                 YAL01460
   16 ANR1=1.                                                        YAL01470
      ANI1=1.                                                        YAL01480
      BNR1=(GM+GP)/ZKR                                               YAL01490
      BNI1=(GM+GP)/ZKI                                               YAL01500
      XFR  =ANR1                                                     YAL01510
      XFI  =ANI1                                                     YAL01520
      XGR  =BNR1                                                     YAL01530
      XGI  =BNI1                                                     YAL01540
   15 DOMR= T  *(  T -2.*SVOFK+2.*ZKR)                               YAL01550
      DOMI=  T *(  T -2.*SVOFK+2.*ZKI)                               YAL01560
      ANR=(-GGP*ANR1-(  T +ZKR)*BNR1)*X1/DOMR                        YAL01570
      BNR=((ZKR+  T -2.*SVOFK)*ANR1-(GM+GP)*BNR1)*X1/DOMR            YAL01580
      ANI=(-GGP*ANI1-(  T +ZKI)*BNI1)*X1/DOMI                        YAL01590
      BNI=((ZKI+  T -2.*SVOFK)*ANI1-(GM+GP)*BNI1)*X1/DOMI            YAL01600
      IF(N-1)13,13,14                                                YAL01610
   13 XFR=XFR+ANR                                                    YAL01620
      XFI=XFI+ANI                                                    YAL01630
      XGR=XGR+BNR                                                    YAL01640
      XGI=XGI+BNI                                                    YAL01650
      N=N+1                                                          YAL01660
      T=T+1.0                                                        YAL01670
      ANR1=ANR                                                       YAL01680
      ANI1=ANI                                                       YAL01690
      BNR1=BNR                                                       YAL01700
      BNI1=BNI                                                       YAL01710
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      GOTO15                                                                    YAL01720
   12 ZKR=SVOFK+PHIK                                                            YAL01730
      ZKI=ALPHA2/(DABS(SVOFK)+PHIK)                                             YAL01740
      GOTO16                                                                    YAL01750
   14 IF((DABS(ANR)+DABS(BNR))/(DABS(XFR)+DABS(XGR))-A(13))17,13,13             YAL01760
   17 IF((DABS(ANI)+DABS(BNI))/(DABS(XFI)+DABS(XGI))-A(13))18,13,13             YAL01770
   18 GO TO JACK,(80,81)                                                        YAL01780
   80 GRP=XFR                                                                   YAL01790
      FRP=XGR                                                                   YAL01800
      FIP=XGI                                                                   YAL01810
      GIP=XFI                                                                   YAL01820
      SVOFK=-SVOFK                                                              YAL01830
      ASSIGN 81 TO JACK                                                         YAL01840
      GO TO 32                                                                  YAL01850
   81 GRNEG=XFR                                                                 YAL01860
      FRNEG=XGR                                                                 YAL01870
      GINEG=XFI                                                                 YAL01880
      FINEG=XGI                                                                 YAL01890
      GR(1)=GRNEG                                                               YAL01900
      GI(1)=GINEG                                                               YAL01910
      FR(1)=FRNEG                                                               YAL01920
      FI(1)=FINEG                                                               YAL01930
      SVOFK=DABS(SVOFK)                                                         YAL01940
C                                                                                1AY1940
C     THE ABOVE STEPS CALCULATE THE VALUES OF THE PRIMED SCRIPT G AND            2AY1940
C     PRIMED SCRIPT F,IN APPENDIX OF RAWITSCHER'S ARTICLE, AT POINT X1.          3AY1940
C     THIS INVOLVES THE USE OF THE GIVEN SERIES EXPANSION FOR THESE              4AY1940
C     QUANTITIES. THE FORMS FOR THE RECURRENCE RELATIONS HAVE BEEN               5AY1940
C     MODIFIED SLIGHTY TO FACILITATE CALCULATION AND TO PREVENT SINGU-           6AY1940
C     LARITIES FROM OCCURING IN THE CONSTANTS USED IN THE EXPANSION.             7AY1940
C     THERE ARE 2 OPTIONS IN THE PROGRAM,DEPENDING ON WHETHER A +OR-             8AY1940
C     SVOFK VALUE IS USED. FOR EACH OF THESE,VALUES MUST BE OBTAINED             9AY1940
C     FOR THE IRREGULAR AND REGULAR SOLUTIONS. THE DETAILS OF THE ABOVE         10AY1940
C     STEPS ARE CONTAINED IN THE NOTES HELD BY PROF. BUSKIRK.                   11AY1940
C                                                                               12AY1940
C     THE VERY DETAILED COMMENTS UP TO THIS POINT WILL HEREAFTER BE             13AY1940
C     GENERALIZED TO WHAT THE END RESULT OF A CERTAIN SEQUENCE OF               14AY1940
C     PROGRAM STEPS IS. THE CORRESPONDENCE BETWEEN COMPUTER STEPS AND           15AY1940
C     THEORY FROM THIS POINT ON IS NOT AT ALL OBVIOUS IN MOST INSTANCES         16AY1940
C     AND A THOROUGH UNDERSTANDING OF THIS PROGRAM WILL REQUIRE ANALYSIS        17AY1940
C     OF NOTES HELD BY PROF. BUSKIRK.                                           18AY1940
C                                                                               19AY1940
C     THE GRF,FRP,GIP,FIP ARE WAVE FUNCTIONS FROM SERIES EXPANSION              20AY1940
C     FOR SVOFK=+AND FOR REGULAR(R) AND IRREGULAR(I) CASES. SIMARILY,           21AY1940
C     THE GR(1),FR(1),GI(1),FI(1) ARE FOR SVOFK=-.                              22AY1940
C                                                                               23AY1940
      9 ASSIGN 200 TO JACK                                                      YAL01950
    207 ASSIGN 37 TO N                                                          YAL01960
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      H2=A(11)/2.                                                          YAL01970
      H210=A(11)**2/12.                                                    YAL01980
      K=1                                                                  YAL01990
      L=2                                                                  YAL02000
      X=A(12)                                                              YAL02010
      A0=-1.-EM1P*EALP*SUM2/SUM3                                           YAL02020
      B0=1.+E1P*EALP*SUM2/SUM3                                             YAL02030
      IF(SVOFK)60,61,61                                                    YAL02040
   61 B1L=B0/(2.*DABS(SVOFK)+1.)                                           YAL02050
      F(1)=X*B1L                                                           YAL02060
      G(1)=1.0                                                             YAL02070
      GOTO62                                                               YAL02080
   60 A1L=A0/(2.*DABS(SVOFK)+1.)                                           YAL02090
      F(1)=1.0                                                             YAL02100
      G(1)=X*A1L                                                           YAL02110
C                                                                           1AY2110
CC    THE ABOVE STEPS CALCULATE THE INITIAL VALUES OF THE RADIAL WAVE       2AY2110
CC    FUNCTIONS AT X=A(12),WHERE A(12) WAS EARLIER STARTING POINT FOR       3AY2110
CC    V(R) CALCULATIONS. THE SERIES EXPANSION USED FOR THE INITIAL          4AY2110
CC    VALUES OF F(1) AND G(1) IS FROM THE ARTICLE BY WOLFGANG BUHRING,      6AY2110
CC    Z. PHYSIK,VOLUME 187,P.183. THE INTERNAL REGION SERIES EXPANSION      6AY2110
CC    IS USED,KEEPING ONLY THE FIRST NON-ZERO TERM IN THE SERIES. THE       7AY2110
CC    VALUE OF THIS TERM FOR F(1) OR G(1) DEPENDS ON THE SIGN OF SVOFK.     8AY2110
C                                                                           9AY2110
   62 EP0=EPHI(1)                                                          YAL02120
      EP1=EPP(1)                                                           YAL02130
   35 DO34J=1,4                                                            YAL02140
      AA(J)=AX(J)                                                          YAL02150
      VP=0                                                                 YAL02160
      VP1=0                                                                YAL02170
   34 BA(J)=B(J)                                                           YAL02180
      V1=(EP0-VP)*EM1P                                                     YAL02190
      V2=(EP0-VP)*E1P                                                      YAL02200
      V1P=(EP1-VP1)*EM1P                                                   YAL02210
      V2P=(EP1-VP1)*E1P                                                    YAL02220
      AX(1)=-SVOFK/X                                                       YAL02230
      AX(2)=1.-V2                                                          YAL02240
      AX(3)=-1.+V1                                                         YAL02250
      AX(4)=SVOFK/X                                                        YAL02260
      B(1)=SVOFK*(SVOFK+1.)/X**2-(1.-V2)*(1.-V1)                           YAL02270
      B(2)=-V2P                                                            YAL02280
      B(3)=V1P                                                             YAL02290
      B(4)=SVOFK*(SVOFK-1.)/X**2-(1.-V1)*(1.-V2)                           YAL02300
      X=X+A(11)                                                            YAL02310
      DO33J=1,4                                                            YAL02320
      AX(J)=AX(J)*H2                                                       YAL02330
   33 B(J)=B(J)*H210                                                       YAL02340
      B(1)=1.+B(1)                                                         YAL02350
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      B(4)=1.+B(4)                                                        YAL02360
      K=K+2                                                               YAL02370
      EPO=EPHI(K)                                                         YAL02380
      EP1=EPP(K)                                                          YAL02390
      GOTON,(37,36)                                                       YAL02400
   37 ASSIGN 36 TO N                                                      YAL02410
      GOTO35                                                              YAL02420
   36 DO38J=1,4                                                           YAL02430
      AM(J)=AA(J)+BA(J)                                                   YAL02440
   38 ANM(J)=B(J)-AX(J)                                                   YAL02450
      DEN=ANM(1)*ANM(4)-ANM(2)*ANM(3)                                     YAL02460
      PM(1)=AM(1)*ANM(4)-AM(3)*ANM(2)                                     YAL02470
      PM(2)=AM(2)*ANM(4)-AM(4)*ANM(2)                                     YAL02480
      PM(3)=AM(3)*ANM(1)-AM(1)*ANM(3)                                     YAL02490
      PM(4)=AM(4)*ANM(1)-AM(2)*ANM(3)                                     YAL02500
      F(L)=(PM(1)*F(L-1)+PM(2)*G(L-1))/DEN                                YAL02510
      G(L)=(PM(3)*F(L-1)+PM(4)*G(L-1))/DEN                                YAL02520
      L=L+1                                                               YAL02530
      IF(X-XO)35,40,40                                                    YAL02540
   40 LMAX=L-1                                                            YAL02550
      IF(LAG-250)691,695,695                                              YAL02560
  695 CONTINUE                                                            YAL02570
  691 GOTOJACK,(200,203)                                                  YAL02580
  200 GPP=G(LMAX)                                                         YAL02590
      FPP=F(LMAX)                                                         YAL02600
      SVOFK=-SVOFK                                                        YAL02610
      ASSIGN 203 TO JACK                                                  YAL02620
      GO TO 207                                                           YAL02630
  203 ASSIGN 204 TO JACK                                                  YAL02640
  205 ASSIGN 47 TO N                                                      YAL02680
C                                                                          1AY2680
C     THE ABOVE STEPS ARE FOR THE INTEGRATION OF THE RADIAL WAVE           2AY2680
C     FUNCTIONS OUT TO THE FITTING RADIUS. THE INTEGRATION PROCEDURE       3AY2680
C     IS THAT OF YENNIE,RAVENHALL,AND WILSON, AND IS OUTLINED IN THE       5AY2680
C     PHYSICAL REVIEW,VOLUME 95,NUMBER 2,P.511. IN RELATION TO THIS,       5AY2680
C     ONLY DERIVATIVES UP TO 2ND WERE USED HERE. THE INTEGRATION IS        6AY2680
C     DONE FOR BOTH +AND- VALUES OF SVOFK. AFTER COMPLETION OF THIS        7AY2680
C     INTEGRATION PROCEDURE, GPP AND FPP WILL CONTAIN FINAL VALUES         8AY2680
C     FOR + SVOFK AND G(LMAX) AND F(LMAX) HAVE VALUES FOR - SVOFK.         9AY2680
C                                                                         10AY2680
      K=1                                                                 YAL02690
      H2=A(11)/2.                                                         YAL02700
      H210=A(11)**2/12.                                                   YAL02710
      X=A(16)                                                             YAL02720
      L=2                                                                 YAL02730
      IF(XO-A(16)-3.*A(11))321,321,45                                     YAL02740
C                                                                          1AY2740
C     AT THIS POINT, A CHECK IS MADE TO DETERMINE IF INTEGRATION OF        2AY2740
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C       COULOMB FUNCTIONS FROM PREVIOUS X1 TO XO IS NECESSARY. THIS IS     3AY2740
C       DETERMINED BY ABOVE IF STATEMENT. DUE TO SPACING USED IN NUMER-    4AY2740
C       ICAL INTEGRATION OF RADIAL WAVE FUNCTIONS,VALUE OF XO, AND VALUE   5AY2740
C       OF X1,FURTHER INTEGRATION MAY BE NECESSARY OVER THIS SMALL RANGE.  6AY2740
C                                                                          7AY2740
  321   LMAXIR=1                                                         YAL02750
        GR(LMAXIR)=GRP                                                   YAL02760
        FR(LMAXIR)=FRP                                                   YAL02770
        GI(LMAXIR)=GIP                                                   YAL02780
        FI(LMAXIR)=FIP                                                   YAL02790
        GRN=GRNEG                                                        YAL02800
        FRN=FRNEG                                                        YAL02810
        GIN=GINEG                                                        YAL02820
        FIN=FINEG                                                        YAL02830
        GO TO 206                                                        YAL02840
C                                                                          1AY2840
CC      INDEPENDENT OF WHETHER FURTHER INTEGRATION IS DONE OR NOT, GR(1),  2AY2840
CC      FR(1),GI(1),AND FI(1) CONTAIN VALUES OF REGULAR AND IRREGULAR      3AY2840
CC      COULOMB WAVE FUNCTIONS FOR + SVOFK. GRN,FRN,FIN,GIN CONTAIN        4AY2840
CC      CORRESPONDING VALUES FOR - SVOFK. IF INTEGRATION IS DONE, THE      5AY2840
CC      RESULTS ARE PUT IN THESE VARIABLE NAMES BY LATER STEPS. THIS       6AY2840
CC      IS NECESSARY SINCE INITIAL SVOFK SIGN IS - FOR FURTHER INTE-       7AY2840
CC      GRATION ROUTINE.                                                   8AY2840
C                                                                          9AY2840
   45   EPO=-EALP/X                                                      YAL02850
        EP1=EALP/X**2                                                    YAL02860
        DO44J=1,4                                                        YAL02870
        AA(J)=AX(J)                                                      YAL02880
   44   BA(J)=B(J)                                                       YAL02890
        V1=(EPO-VP)*EM1P                                                 YAL02900
        V2=(EPO-VP)*E1P                                                  YAL02910
        V1P=(EP1-VP1)*EM1P                                               YAL02920
        V2P=(EP1-VP1)*E1P                                                YAL02930
        AX(1)=-SVOFK/X                                                   YAL02940
        AX(2)=1.-V2                                                      YAL02950
        AX(3)=-1.+V1                                                     YAL02960
        AX(4)=SVOFK/X                                                    YAL02970
        B(1)=SVOFK*(SVOFK+1.)/X**2-(1.-V2)*(1.-V1)                       YAL02980
        B(2)=-V2P                                                        YAL02990
        B(3)=V1P                                                         YAL03000
        B(4)=SVOFK*(SVOFK-1.)/X**2-(1.-V1)*(1.-V2)                       YAL03010
        X=X+A(11)                                                        YAL03020
        DO43J=1,4                                                        YAL03030
        AX(J)=AX(J)*H2                                                   YAL03040
   43   B(J)=B(J)*H210                                                   YAL03050
        B(1)=1.+B(1)                                                     YAL03060
        B(4)=1.+B(4)                                                     YAL03070
        GOTON,(47,46)                                                    YAL03080
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   47 ASSIGN 46 TO N                                                    YAL03090
      GO TO 45                                                          YAL03100
   46 DO48J=1,4                                                         YAL03110
      AM(J)=AA(J)+BA(J)                                                 YAL03120
   48 ANM(J)=B(J)-AX(J)                                                 YAL03130
      DEN=ANM(1)*ANM(4)-ANM(2)*ANM(3)                                   YAL03140
      PM(1)=AM(1)*ANM(4)-AM(3)*ANM(2)                                   YAL03150
      PM(2)=AM(2)*ANM(4)-AM(4)*ANM(2)                                   YAL03160
      PM(3)=AM(3)*ANM(1)-AM(1)*ANM(3)                                   YAL03170
      PM(4)=AM(4)*ANM(1)-AM(2)*ANM(3)                                   YAL03180
      FR(L)=(PM(1)*FR(L-1)+PM(2)*GR(L-1))/DEN                           YAL03190
      GR(L)=(PM(3)*FR(L-1)+PM(4)*GR(L-1))/DEN                           YAL03200
      FI(L)=(PM(1)*FI(L-1)+PM(2)*GI(L-1))/DEN                           YAL03210
      GI(L)=(PM(3)*FI(L-1)+PM(4)*GI(L-1))/DEN                           YAL03220
      L=L+1                                                             YAL03230
      IF(X-X0)45,50,50                                                  YAL03240
   50 LMAXIR=L-1                                                        YAL03250
      GO TO JACK,(204,206)                                              YAL03260
  204 GRN=GR(LMAXIR)                                                    YAL03270
      GIN=GI(LMAXIR)                                                    YAL03280
      FRN=FR(LMAXIR)                                                    YAL03290
      FIN=FI(LMAXIR)                                                    YAL03300
      GR(1)=GRP                                                         YAL03310
      GI(1)=GIP                                                         YAL03320
      FR(1)=FRP                                                         YAL03330
      FI(1)=FIP                                                         YAL03340
      SVOFK=DABS(SVOFK)                                                 YAL03350
      ASSIGN 206 TO JACK                                                YAL03360
      GO TO 205                                                         YAL03370
C                                                                        1AY3370
CCC   THE ABOVE STEPS ARE FOR THE INTEGRATION, IF NECESSARY, OF THE      2AY3370
CCC   COULOMB WAVE FUNCTIONS. THE INTEGRATION PROCEDURE IS THE SAME      3AY3370
CCC   AS WAS EARLIER USED FOR RADIAL WAVE FUNCTIONS. THE ONLY MAJOR      4AY3370
CCC   DIFFERENCE IS THAT THE POTENTIAL USED HERE IS THAT FOR A POINT     5AY3370
CCC   NUCLEUS.                                                          6AY3370
C                                                                        7AY3370
  206 STEAM=DEXP(GAM1(PHIK,GM)-GAM1(2.0*PHIK,0)+PHIK*DLOG(A(16)))       YAL03380
      TYRE=STEAM**2                                                     YAL03420
      TEMP=   TYRE*(                                                    YAL03430
     1SQRT(SQS(PHIK,GM))/(2.*PHIK))*(DSQRT((CSHY(3.141593*GM))**2-(DCO  YAL03440
     2S (3.141593*PHIK))**2)/DSIN(6.283185*PHIK))                       YAL03450
      TEMP1=((GM+GP)*(DABS(SVOFK)+PHIK)/((DABS(SVOFK)*GM-GP*PHIK)*ALPHA2YAL03460
     1))*(DABS(SVOFK)*(DABS(SVOFK)+PHIK)-GP*ALPHA2/(GM+GP))             YAL03470
      SVOFK=DABS(SVOFK)                                                 YAL03480
      RNINP=TEMP*SQRT(TEMP1)*2.**(2.*PHIK)                              YAL03490
      RNINN=(TEMP/SQRT(TEMP1))*2.**(2.*PHIK)                            YAL03500
      ASSIGN 800 TO JACK                                                YAL03510
      DCKP=((GR(LMAXIR)-(GPP/FPP)*FR(LMAXIR))/((GPP/FPP)*FI(LMAXIR)-GI( YAL03520
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     1LMAXIR)))*RNINP                                                          YAL03530
      DCKN=((GRN-(G(LMAX)/F(LMAX))*FRN)/((G(LMAX)/F(LMAX))*FIN-GIN))*          YAL03540
     1RNINN                                                                    YAL03550
C                                                                               1AY3550
CCC    THE ABOVE STEPS CALCULATE THE RATIO(D/C),WHERE D AND C ARE THE           2AY3550
CCC    MATCHING COEFFICIENTS USED IN THE MATCHING OF THE RADIAL WAVE            3AY3550
CCC    FUNCTIONS AND THE REGULAR AND IRREGULAR COULOMB WAVE FUNCTIONS           4AY3550
CCC    AT THE FITTING RADIUS. THE FORMULA FOR THIS RATIO IS CONTAINED           5AY3550
CCC    IN THE APPENDIX OF RAWITSCHERS ARTICLE. THIS CALUCLATION REQUIRES        6AY3550
CCC    THE RATIO OF THE NORMALIZATION CONSTANTS OF THE POINT COULOMB            7AY3550
CCC    RADIAL WAVES. THE FORMULA FOR THE NORMALIZATION CONSTANTS IS             8AY3550
CCC    GIVEN IN THE APPENDIX. THE FUNCTION GAM1 USED IN THE VARIABLE            9AY3550
CCC    STEAM IS EQUAL TO THE REAL PART OF THE NATURAL LOG OF THE GAMMA          10AY3550
CCC    FUNCTION(X+IY),WHERE I IS IMAGINARY I.I.E.,SQUARE ROOT OF -1. GAM1       11AY3550
CCC    IS FOR CALCULATING VALUES OF GAMMA FUNCTIONS IN THE NORMALIZATION        12AY3550
CCC    CONSTANTS RATIO FORMULA.                                                 13AY3550
C                                                                               14AY3550
  901 IF((1.+PHIK)-3.)951,953,953                                               YAL03590
  951 XR=(3.141593/2.)*(DABS(SVOFK)-1.-PHIK)-GAM4(PHIK+1.,GM)                   YAL03600
      GO TO 998                                                                 YAL03610
  953 XR=(3.141593/2.)*(DABS(SVOFK)-1.-PHIK)-GAM3(PHIK+1.,GM)                   YAL03620
  998 IF(1.-PHIK)54,55,55                                                       YAL03630
   54 IF((PHIK+1.)-3.)957,963,963                                               YAL03640
  957 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-(GAM4(PHIK+1.,GM)-DATAN(GM        YAL03650
     1/PHIK))                                                                   YAL03660
      U=DSIN(3.141593*(1.0-PHIK))*CSHY(3.141593*GM)                             YAL03670
      V=DCOS(3.141593*(1.-PHIK))*SSHY(3.141593*GM)                              YAL03680
      IF(U)56,57,57                                                             YAL03690
   57 ARG=ATAN(V/ABS(U))                                                        YAL03700
      GO TO 58                                                                  YAL03710
   56 ARG=(3.141593-ATAN(ABS(V)/ABS(U)))*V/ABS(V)                               YAL03720
   58 XI=XI+ARG                                                                 YAL03730
      GO TO 91                                                                  YAL03740
   55 IF((1.-PHIK)-3.)59,90,90                                                  YAL03750
   59 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-GAM4((-PHIK+1.),GM)                YAL03760
      GO TO 91                                                                  YAL03770
   90 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-GAM3((-PHIK+1.),GM)                YAL03780
      GO TO 91                                                                  YAL03790
  963 XI=(3.141593/2.)*(DABS(SVOFK)-1.+PHIK)-(GAM3(PHIK+1.,GM)-DATAN(GM        YAL03800
     1/PHIK))                                                                   YAL03810
      U=DSIN(3.141593*(1.0-PHIK))*CSHY(3.141593*GM)                             YAL03820
      V=DCOS(3.141593*(1.-PHIK))*SSHY(3.141593*GM)                              YAL03830
      IF(U) 751,752,752                                                         YAL03840
  751 ARG=(3.141593-ATAN(ABS(V)/ABS(U)))*V/ABS(V)                               YAL03850
      GO TO 58                                                                  YAL03860
  752 ARG=ATAN(V/ABS(U))                                                        YAL03870
      GO TO 58                                                                  YAL03880
   91 SRY=-A(8)*((SVOFK*(SVOFK+PHIK)+GP*(GP-GM))/(2.*SQS(SVOFK,GP)))**.         YAL03890
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15                                                                      YAL03900
 CRY=((SVOFK*(SVOFK-PHIK)+GP*(GP+GM))/(2.*SQS(SVOFK,GP)))**.5           YAL03910
 SRYI=A(8)*((SVOFK*(SVOFK-PHIK)+GP*(GP-GM))/(2.*SQS(SVOFK,GP)))**.      YAL03920
15                                                                      YAL03930
 CRYI=((SVOFK*(SVOFK+PHIK)+GP*(GP+GM))/(2.*SQS(SVOFK,GP)))**.5          YAL03940
 SNKR=SIN(XR)*CRY+SRY*COS(XR)                                           YAL03950
 CNKR=COS(XR)*CRY-SIN(XR)*SRY                                           YAL03960
 SNKI=COS(XR)*CRYI-SIN(XR)*SRYI                                         YAL03970
 CNKI=-SIN(XR)*CRYI-SRYI*COS(XR)                                        YAL03980
 SKR=SIN(XI)*CRYI-SRYI*COS(XI)                                          YAL03990
 CKR=COS(XI)*CRYI+SIN(XI)*SRYI                                          YAL04000
 SKI=COS(XI)*CRY+SRY*SIN(XI)                                            YAL04010
 CKI=-SIN(XI)*CRY+COS(XI)*SRY                                           YAL04020
 TNKP=(SNKR+DCKP*SKR)/(CNKR+DCKP*CKR)                                   YAL04030
 C2NKP=(1.-TNKP**2)/(1.+TNKP**2)                                        YAL04040
 S2NKP=2.*TNKP/(1.+TNKP**2)                                             YAL04050
 TNKRP=SNKR/CNKR                                                        YAL04060
 CNRP=(1.-TNKRP**2)/(1.+TNKRP**2)                                       YAL04070
 SNRP=2.*TNKRP/(1.+TNKRP**2)                                            YAL04080
 TNKM=(SNKI+DCKN*SKI)/(CNKI+DCKN*CKI)                                   YAL04090
 C2KM=(1.-TNKM**2)/(1.+TNKM**2)                                         YAL04100
 S2KM=2.*TNKM/(1.+TNKM**2)                                              YAL04110
 TKRM=SNKI/CNKI                                                         YAL04120
 CNRM=(1.-TKRM**2)/(1.+TKRM**2)                                         YAL04130
 SNRM=2.*TKRM/(1.+TKRM**2)                                              YAL04140
 TKR=SKR/CKR                                                            YAL04150
 TKI=SKI/CKI                                                            YAL04160
 ATA(LOP)=ATAN(TKR)                                                     YAL04170
 ETI(LOP)=ATAN(TKI)                                                     YAL04180
 ETAKP(LOP)=ATAN(TNKRP)                                                 YAL04190
 ETAKN(LOP)=ATAN(TKRM)                                                  YAL04200
 ETKP(LOP)=ATAN(TNKP)                                                   YAL04210
 ETKN(LOP)=ATAN(TNKM)                                                   YAL04220
C                                                                        1AY4220
CC   ALL OF THE ABOVE STEPS ARE CONCERNED WITH THE CALCULATION OF        2AY4220
CC   6 NEEDED PHASE SHIFTS, SUMMARIZED BELOW:                           3AY4220
CC   ATA=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=+                      4AY4220
CC   ETI=IRREGULAR COULOMB PHASE SHIFT FOR SVOFK=-                      5AY4220
CC   ETAKP=REGULAR COULOMB PHASE SHIFT FOR SVOFK=+                      6AY4220
CC   ETAKN=REGULAR COULOMB PHASE SHIFT FOR SVOFK=-                      7AY4220
CC   ETKP=NUCLEAR PHASE SHIFT FOR SVOFK=+                               8AY4220
CC   ETKN=NUCLEAR PHASE SHIFT FOR SVOFK=-                               9AY4220
CC   THE MANY STEPS USED ARE BASED ON THE FORMULA FOR THE PHASE SHIFTS  10AY4220
CC   GIVEN IN THE APPENDIX. THE MATHEMATICAL BASIS FOR THE ABOVE STEPS  11AY4220
CC   IS CONTAINED IN THE NOTES HELD BY PROF. BUSKIRK. THE GAM3 AND      12AY4220
CC   GAM4 FUNCTIONS ARE USED IN CALCULATING THE ARGUMENT OF GAMMA FUNC-13AY4220
CC   TIONS CONTAINED IN APPLICABLE FORMULAS.                           14AY4220
C                                                                       15AY4220
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      IF(ABS(ATA(LOP)).LE.(1.0E-50)) ATA(LOP)=0.0                       YAL04230
      IF(ABS(ETI(LOP)).LE.(1.0D-50)) ETI(LOP)=0.0                       YAL04240
      IF(ABS(ETAKP(LOP)).LE.(1.0E-50))ETAKP(LOP)=0.0                    YAL04250
      IF(ABS(ETAKN(LOP)).LE.(1.0E-50))ETAKN(LOP)=0.0                    YAL04260
      IF(ABS(ETKP(LOP)).LE.(1.0E-50)) ETKP(LOP)=0.0                     YAL04270
      IF(ABS(ETKN(LOP)).LE.(1.0E-50)) ETKN(LOP)=0.0                     YAL04280
      GO TO JACK ,(800,801)                                             YAL04290
  800 Q=2.-SNRP*S2NKP-CNRP*C2NKP-S2KM*SNRM-C2KM*CNRM                    YAL04300
      TEST=DCKP**2+Q                                                    YAL04340
      IF(TEST-A(14))100,101,101                                         YAL04350
C                                                                        1AY4350
CCC   REFERENCE TO DETAILED NOTES WILL VERIFY THAT AS THE VALUE OF TEST  2AY4350
CCC   APPROACHES ZERO THE NUCLEAR PHASE SHIFT APPROACHES THE REGULAR     3AY4350
CCC   COULOMB PHASE SHIFT VALUE.                                         4AY4350
C                                                                        5AY4350
  101 SVFKM=-SVOFK                                                      YAL04360
      SVOFK=DABS(SVOFK)+1.000000000000                                  YAL04370
      LOP=LOP+1                                                         YAL04380
      GO TO 10                                                          YAL04390
C                                                                        1AY4390
CCC   IF THE VALUE OF TEST-A(14),WHERE A(14) IS PRESENTLY 0.1D-09,IS     2AY4390
CCC   GREATER THAN ZERO, THEN THE ANGULAR MOMENTUM QUANTUM NUMBER IS     3AY4390
CCC   INCREASED BY 1 AND RETURN TO RECALCULATION OF COULOMB FUNCTIONS    5AY4390
CCC   TAKES PLACE. ALL CALCULATIONS ARE THUS REDONE FOR NEW VALUE OF     5AY4390
CCC   SVOFK.                                                            6AY4390
C                                                                        7AY4390
  100 ASSIGN 801 TO JACK                                                YAL04400
  801 SVOFK=DABS(SVOFK)+1.000000000000                                  YAL04410
      PHIK=DSQRT(SVOFK**2-ALPHA2)                                       YAL04420
      IF(LOP-LAG) 905,905,105                                           YAL04430
C                                                                        1AY4430
CCC   THE ABOVE STEP TERMINATES CALCULATION OF PHASE SHIFTS WHEN SVOFK   2AY4430
CCC   REACHES VALUE OF LAG. LAG IS SET AT 34 NOW, BUT COULD BE CHANGED   3AY4430
CCC   IF DESIRED. THE VALUE OF LAG DOES NOT AFFECT THE POINT AT WHICH    4AY4430
CCC   NUCLEAR PHASE SHIFTS ARE SET EQUAL TO COULOMB,UNLESS SVOFK VALUE   5AY4430
CCC   EQUAL TO LAG IS REACHED BEFORE TRANSFER TO COULOMB OCCURS. FOR     6AY4430
CCC   INCIDENT ENERGIES LESS THAN 500 MEV,TRANSFER TO COULOMB FUNCTIONS  7AY4430
CCC   WILL OCCUR BEFORE SVOFK=34. FOR HIGH ENERGIES, IT MAY BE DESIRABLE 8AY4430
CCC   TO USE LARGER LAG VALUE TO ENSURE INCLUSION OF ENOUGH VALUES OF    9AY4430
CCC   SVOFK.                                                           10AY4430
C                                                                       11AY4430
  905 ETKP(LOP)=ETAKP(LOP)                                              YAL04440
      ETKN(LOP)=ETAKN(LOP)                                              YAL04450
      LOP=LOP+1                                                         YAL04470
      GO TO 901                                                         YAL04480
  105 CONTINUE                                                          YAL04490
      ETKP(LOP) = ETAKP(LOP)                                            YAL04500
      ETKN(LOP) = ETAKN(LOP)                                            YAL04510
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C                                                                       1AY4510
C     THE CALCULATION OF PHASE SHIFTS IS COMPLETE AND THE SUMMATION OF  2AY4510
C     LEGENDRE POLYNOMIALS IS DONE NEXT TO GET SCATTERING AMPLITUDES.   3AY4510
C                                                                       4AY4510
  108 KMAX=LOP                                                        YAL04550
      K=1                                                             YAL04560
      M=1                                                             YAL04570
      SVOFK=0                                                         YAL04580
      DO 166JOG=1,LOP                                                 YAL04590
      IF(K.EQ.1) GO TO 165                                            YAL04600
      ALR(JOG)=COS(2.*ETKN(K-1))-COS(2.*ETKP(K))                      YAL04610
      ALI(JOG)=SIN(2.*ETKN(K-1))-SIN(2.*ETKP(K))                      YAL04620
      GO TO 166                                                       YAL04630
  165 ALR(JOG)=-COS(2.*ETKP(K))                                       YAL04640
      ALI(JOG)=-SIN(2.*ETKP(K))                                       YAL04650
  166 K=K+1                                                           YAL04660
      K=1                                                             YAL04670
      SVOFK=0.0                                                       YAL04680
      N=LOP-1                                                         YAL04690
      DO111J=1,N                                                      YAL04700
      TEMP=(SVOFK+1.)*(SVOFK+2.)/(2.*SVOFK+3.)                        YAL04710
      TEMP1=SVOFK*(SVOFK-1.)/(2.*SVOFK-1.)                            YAL04720
      IF(K.EQ.1) GO TO 110                                            YAL04730
      COR(J,1)=(SVOFK+1.)*COS(2.*ETKP(K))+SVOFK*COS(2.*ETKN(K-1))     YAL04740
      COR(J,1)=COR(J,1)-(2.0*SVOFK+1.0)                               YAL04750
      COI(J,1)=(SVOFK+1.)*SIN(2.*ETKP(K))+SVOFK*SIN(2.*ETKN(K-1))     YAL04760
      DOR(J,1)=TEMP*ALR(K+1)-TEMP1*ALR(K-1)                           YAL04780
      DOI(J,1)=TEMP*ALI(K+1)-TEMP1*ALI(K-1)                           YAL04790
      JM=J-1                                                          YAL04800
      GO TO 993                                                       YAL04820
  110 COR(J,1)=(SVOFK+1.)*COS(2.*ETKP(K))                             YAL04830
      COR(J,1)=COR(J,1)-(2.0*SVOFK+1.0)                               YAL04840
      COI(J,1)=(SVOFK+1.)*SIN(2.*ETKP(K))                             YAL04850
      DOR(J,1)=TEMP*ALR(K+1)                                          YAL04860
      DOI(J,1)=TEMP*ALI(K+1)                                          YAL04870
      JM=J-1                                                          YAL04880
  993 K=K+1                                                           YAL04900
  111 SVOFK=SVOFK+1.                                                  YAL04910
C                                                                       1AY4910
C     THE ABOVE STEPS CALCULATE THE COEFFICIENTS C AND D CONTAINED IN   2AY4910
C     THE EXPRESSIONS FOR THE SCATTERING AMPLITUDES,WHICH ARE GIVEN     3AY4910
C     IN THE APPENDIX.                                                  4AY4910
C                                                                       5AY4910
  112 K=1                                                             YAL04950
      N=LOP-1-M                                                       YAL04960
      SVOFK=0                                                         YAL04970
      DO128J=1,N                                                      YAL04980
      IF(K.EQ.1) GO TO 1128                                           YAL04990
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      COR(J,M+1)=COR(K,M)-(SVOFK+1.)*COR(K+1,M)/(2.*SVOFK+3.)-SVOFK*COR(YAL05000
     1K-1,M)/(2.*SVOFK-1.)                                                YAL05010
      COI(J,M+1)=COI(K,M)-(SVOFK+1.)*COI(K+1,M)/(2.*SVOFK+3.)-SVOFK*COI(YAL05020
     1K-1,M)/(2.*SVOFK-1.)                                                YAL05030
      DOR(J,M+1)=DOR(K,M)-(SVOFK+1.)*DOR(K+1,M)/(2.*SVOFK+3.)-SVOFK*DOR(YAL05040
     1K-1,M)/(2.*SVOFK-1.)                                                YAL05050
      DOI(J,M+1)=DOI(K,M)-(SVOFK+1.)*DOI(K+1,M)/(2.*SVOFK+3.)-SVOFK*DOI(YAL05060
     1K-1,M)/(2.*SVOFK-1.)                                                YAL05070
      K=K+1                                                               YAL05080
      GO TO 128                                                           YAL05090
 1128 COR(J,M+1)=COR(K,M)-(SVOFK+1.)*COR(K+1,M)/(2.*SVOFK+3.)             YAL05100
      COI(J,M+1)=COI(K,M)-(SVOFK+1.)*COI(K+1,M)/(2.*SVOFK+3.)             YAL05110
      DOR(J,M+1)=DOR(K,M)-(SVOFK+1.)*DOR(K+1,M)/(2.*SVOFK+3.)             YAL05120
      DOI(J,M+1)=DOI(K,M)-(SVOFK+1.)*DOI(K+1,M)/(2.*SVOFK+3.)             YAL05130
      K=K+1                                                               YAL05140
  128 SVOFK=SVOFK+1.                                                      YAL05150
      M=M+1                                                               YAL05160
      IF(M-5)112,135,135                                                  YAL05170
  135 CONTINUE                                                            YAL05180
C                                                                          1AY5180
CCCCC THE ABOVE STEPS CALCULATE THE VALUES OF THE COEFFICIENTS PERTINENT   2AY5180
CCCCC TO METHOD OF SUMMATION OF LEGENDRE POLYNOMIALS BY REDUCED COEF-      3AY5180
CCCCC FICIENTS. FOURTH ORDER REDUCED COEFFICIENTS ARE USED IN THIS         4AY5180
CCCCC METHOD IN THIS PROGRAM.                                              5AY5180
C                                                                          6AY5180
      ITHXX = 0                                                           YAL05220
      EINCX=EINCX+0.511                                                   YAL05230
      A(3)=EINCX                                                          YAL05240
  113 I=KMAX-5                                                            YAL05250
      ITHXX = ITHXX + 1                                                   YAL05260
      THETA=THEXX(ITHXX)/57.29578                                         YAL05270
      SVOFK=0                                                             YAL05280
      ZP(1)=1.                                                            YAL05290
      ZP(2)=COS(THETA)                                                    YAL05300
      DO114J=3,I                                                          YAL05310
      SVOFK=SVOFK+1.                                                      YAL05320
  114 ZP(J)=((2.*SVOFK+1.)*COS(THETA)*ZP(J-1)-SVOFK*ZP(J-2))/(SVOFK+1.)   YAL05330
      I=KMAX-5                                                            YAL05340
      SVOFK=0                                                             YAL05350
      FTH=0                                                               YAL05360
      FTI=0                                                               YAL05370
      GTH=0                                                               YAL05380
      GTI=0                                                               YAL05390
      DF=2.*CK*(1.-COS(THETA))**4                                         YAL05400
      DG=DF*SIN(THETA)                                                    YAL05410
      DO115K=1,I                                                          YAL05420
      FTH=FTH+COR(K,5)*ZP(K)                                              YAL05430
      GTH=GTH+DOR(K,5)*ZP(K)                                              YAL05440
```

```
      FTI=FTI+COI(K,5)*ZP(K)                                                YAL05450
  115 GTI=GTI+DOI(K,5)*ZP(K)                                                YAL05460
      FTH=-FTH/DF                                                           YAL05470
      FTI=FTI/DF                                                            YAL05480
      GTH=-GTH/DG                                                           YAL05490
      GTI=GTI/DG                                                            YAL05500
      SIG=FTH**2+FTI**2+GTH**2+GTI**2                                       YAL05510
      STH=-2.*(FTH*GTI-FTI*GTH)/SIG                                         YAL05520
      OMAG = THETA/2.0                                                      YAL05530
      SIM =SIN(OMAG)                                                        YAL05540
      CONST1=(A(2)*A(9))/2.0                                                YAL05550
      SIGMT=((CONST1**2)*(1.0-(BETA*SIM)**2))/(((BETA*CK)**2)*SIM**4)       YAL05560
      FELS=SIG/SIGMT                                                        YAL05570
      SIGTXX(ITHXX)=SIG                                                     YAL05580
      SIGMTX(ITHXX)=SIGMT                                                   YAL05590
      FELSXX(ITHXX)=FELS                                                    YAL05600
      MXXDYX=ITHXX-LXXXXX                                                   YAL05610
      IF(MXXDYX)113,6969,6969                                               YAL05620
C                                                                            1AY5620
CCCC  IN THE ABOVE STEPS, SIG=EXACT CROSS SECTION, AND SIGMT=MOTT POINT     2AY5620
CCCC  NUCLEUS CROSS SECTION. THE SUMMATION OF LEGENDRE POLYNOMIALS          3AY5620
CCCC  ALSO IS DONE ABOVE TO GET REAL AND IMAGINARY PARTS OF SCATTERING      4AY5620
CCCC  AMPLITUDES; FTH,GTH,AND FTI, GTI RESPECTIVELY.                        5AY5620
C                                                                            6AY5620
 6969 CONTINUE                                                              YAL05630
      RETURN                                                                YAL05640
      END                                                                   YAL05650
C                                                                            1AY5650
CCCC  THE FOLLOWING IS THE FUNCTION FMOD WHERE THE CHARGE DENSITY FOR       2AY5650
CCCC  A GIVEN RADIAL DISTANCE IS CALCULATED. THERE ARE PRESENTLY 5          3AY5650
CCCC  MODELS HERE AND THE SELECTION IS BASED ON INPUT PARAMETER MODEL,      4AY5650
CCCC  AS WAS MENTIONED EARLIER. TO ADD ADDITIONAL MODELS IT IS ONLY         5AY5650
CCCC  NECESSARY TO CHANGE INITIAL GO TO STATEMENT AND SUPPLY APPROPRIATE    6AY5650
CCC   CARDS.                                                                7AY5650
C                                                                            8AY5650


      FUNCTION FMOD(MODEL,RX,CK,C,TXXXX,WXXXX)                              YAL05660
      GO TO (1,2,3,4,5),MODEL
    1 CP=C*CK                                                               YAL05680
      TP=TXXXX*CK/4.3944                                                    YAL05690
      FMOD=1.0/(1.0+EXP((RX-CP)/TP))                                        YAL05700
      RETURN                                                                YAL05710
C                                                                            1AY5710
CCC   #1 IS A FERMI CHARGE DISTRIBUTION.                                     2AY5710
C                                                                            3AY5710
    2 CP=C*CK                                                               YAL05720
      TP=TXXXX                                                              YAL05730
```

```
      FMOD=(1.0+TP*(RX/CP)**2)*EXP(-(RX/CP)**2)                          YAL05740
      RETURN                                                             YAL05750
C                                                                         1AY5750
CCC   #2 IS A GAUSSIAN P-SHELL CHARGE DISTRIBUTION.                       2AY5750
C                                                                         3AY5750
    3 C=2.12                                                             YAL05760
      C=C*CK                                                             YAL05770
      FMOD= EXP(-(RX/C)**2)                                              YAL05780
      RETURN                                                             YAL05790
C                                                                         1AY5790
CCC   #3 IS A GAUSSIAN CHARGE DISTRIBUTION.                               2AY5790
C                                                                         3AY5790
    4 ALIT=0.0019                                                        YAL05800
      BLIT=(4.4)*CK                                                      YAL05810
      CLIT=(1.1)*CK                                                      YAL05820
      ABIG=(1.649)*CK                                                    YAL05830
      BBIG=(1.705)*CK                                                    YAL05840
      FMOD=(1.0+(RX/BBIG)**2)*EXP(-(RX/ABIG)**2)+ALIT*EXP(-(RX-BLIT)**2/YAL05840
     1CLIT**2)                                                           YAL05850
      RETURN                                                             YAL05860
C                                                                         1AY5860
CCC   #4 IS A CARBON-12 CHARGE DISTRIBUTION DEVELOPED FROM WORK AT        2AY5860
      STANFORD BUT PRESENTLY CONSIDERED NOT CORRECT.                      3AY5860
C                                                                         4AY5860
    5 ASMAL=(0.932)*CK                                                   YAL05870
      BSMAL=(1.305)*CK                                                   YAL05880
      CSMAL2=(0.335)*((CK)**2)                                           YAL05890
      FMOD=(1.0/(8.0*((3.14159)**1.5)))*((1.0/ASMAL**3)*EXP(-(RX/(2.0*ASYAL05900
     1MAL))**2)-(CSMAL2*(6.0*(BSMAL**2)-(RX**2))/(4.0*(BSMAL**7)))       YAL05910
     2*EXP(-(RX/(2.0*BSMAL))**2))                                        YAL05920
      RETURN                                                             YAL05930
C                                                                         1AY5930
CCC   #5 IS A LITHIUM-6 CHARGE DISTRIBUTION DEVELOPED BY SUELZLE.         2AY5930
C                                                                         3AY5930
      END                                                                YAL05770
```

BIBLIOGRAPHY

1. Hofstader, R., Fechter, H. R., and McIntyre, J. A., Phys. Rev., volume 91, p. 422, 1953; volume 92, p. 778, 1953.

2. Pidd, R. W., Hammer, C. L., and Raka, E. C., Phys. Rev., volume 92, p.436, 1953.

3. Yennie, D R., Ravenhall, D. G., and Wilson, R. N., Phys. Rev., volume 95, p. 500, 1954.

4. Rawitscher, G. H., Phys. Rev., volume 112, p. 1274, 1958.

5. Mott, N. F., and Massey, H. S. W., The Theory of Atomic Collisions, 2nd ed., Ch. 4, Sec. 4., Clarendon Press, 1949.

6. Schiff, L I., Phys. Rev., volume 92, p. 988, 1953.

7. Suelzle, L. R., Yearian, M. R., and Crannel, H., Phys. Rev., volume 162, p. 992, 1967.

8. Schiff, L. I., Quantum Mechanics, E. 44.10, McGraw Hill, 1949.

9. Milne, W. E., Numerical Solution of Differential Equations, p. 76-78, John Wiley and Sons, 1953.

10. Burring, W., Z. Physik, volume 192, p. 13, 1966.

11. Dedrick, K. G., Rev. Mod. Phys., volume 34, p. 429, 1962.

12. Whittaker, E. T., and Watson, G. N., A Course of Modern Analysis, 4th ed., Ch. 12, Cambridge University Press, 1927.

13. Monson, W. A., Measurement of Lithium-6 Charge Form Factors, Thesis, Naval Postgraduate School, 1969.

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13. ABSTRACT

A phase shift analysis is used to obtain scattering across sections for incident electrons on Carbon-12 and Lithium-6. Results are given for incident electron energies of 10 - 100 Mev and for scattering angles of 45, 90 and 135 degrees. A gaussian p-shell charge distribution is used for Carbon-12, and an empirical charge distribution developed by L. R. Suelzle is used for Lithium-6. A comparison is also made between the phase-shift results and results obtained using the Born approximation.

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